Major Shared Resource Center

ERDC MSRC

Programming Environment and Training Annual Report - Year Five

2000 - 2001

Work funded by the Department of Defense
High Performance Computing Modernization Program
U.S. Army Engineer Research and Development Center
Major Shared Resource Center through

Programming Environment and Training

Supported by Contract Number: DAHC94-96-C0002
Computer Sciences Corporation

TABLE OF CONTENTS

LIST OF TABLES

EXECUTIVE SUMMARY

The true deliverable of the U.S. Army Engineer Research and Development Center (ERDC) Major Shared Resource Center (MSRC) Programming Environment and Training (PET) effort is the raised level of ERDC MSRC user capability and programming environment in the ERDC MSRC - to a level unsurpassed by academic, industry, or other government HPC centers. The ERDC MSRC PET team addresses this charge by providing core support to ERDC MSRC users, performing specific focused efforts designed to introduce new tools and computational technology into the ERDC MSRC, conducting training courses and workshops for ERDC MSRC users, and operating an HBCU/MI (MSI) enhancement program.

The PET component of the DoD HPC MSRCs is a bold and innovative university/industry/government effort providing the essential user support and mode of capability enhancement necessary for the MSRCs to reach a level comparable to that in the foremost university, industry, and other Government agency HPC centers - and to address the wide variety of research and development demands arising from the science and technology programs supporting DoD's weapons development and warfighting support systems. The purpose of the PET component of the MSRCs is to enhance the entire programming environment for the MSRC users through training and support for software enhancement, addressing both near-term improvements and long-term expansions, thus enabling use of the MSRC computing resources to fullest capacity and extending the range of applicability of HPC to DoD technical problems.

The PET effort is unprecedented in its concept and vision, management for long-term achievement, strong university commitment, approach through unique university/DoD collaboration, in its understanding and relationship between university researchers and MSRC users - and in its challenge to be faced in the interest of DoD by the universities and companies involved, the MSRC users, and the program management. The PET component of the MSRC program is truly an intellectual enterprise that breaks new ground in collaborative effort between DoD and academia in order to establish a two-way conduit of information and expertise enhancing the capability of the MSRC user and bringing demands of DoD HPC to bear early-on in programming environment developments in progress in the universities.

The ERDC MSRC PET effort is administered by the integrator, Computer Sciences Corporation (Nichols Research) for the ERDC MSRC as a part of the contract for the ERDC MSRC. Dr. Henry Gabb of CSC was the PET Director during part of Year 5, followed by John West. Dr. Joe Thompson of Mississippi State University is the ERDC MSRC PET academic team leader. Dr. Wayne Mastin of CSC, also a professor emeritus at Mississippi State, is the on-site PET team leader. Dr. Willie Brown of Jackson State University is the HBCU/MI leader. Dr. Louis Turcotte of the ERDC MSRC exercised oversight of the ERDC MSRC PET effort for the government for part of Year 5, followed by Bob Athow.

The fundamental mode of operation for PET at the ERDC MSRC is a direct and continual connection between the ERDC MSRC users and the ERDC MSRC PET team universities in support of five Computational Technology Areas (CTAs) supported at the ERDC MSRC and three related technical infrastructure areas. This is accomplished through a combination of full-time university and CSC personnel on-site at the ERDC MSRC, in close communication with dedicated university personnel dividing time between the ERDC MSRC and the university, and with faculty members at the university with partial commitment to the ERDC MSRC PET effort for support and leadership.

The university PET team for the ERDC MSRC is led by the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University, with Jackson State University as the lead HBCU/MI. The university team is as follows:

- Center for Computational Field Simulation
  (*NSF Engineering Research Center at Mississippi State*)

- National Center for Supercomputing Applications - NCSA
  (*NSF PACI Center at Illinois*)

- Ohio State University and Ohio Supercomputer Center - OSC
  (*at Ohio State*)

- Texas Institute for Computational and Applied Mathematics – TICAM
  (at Texas)

- Syracuse University

- Florida State University

- Rice University

- University of Tennessee

- University of Texas at Arlington

- HBCU/MIs: Jackson State University, Clark Atlanta University, and Texas A&M University-Kingsville

Dedicated on-site/at-university support teams for each of the five DoD Computational Technology Areas (CTAs) supported at the ERDC MSRC were the responsibility of specific universities on the PET team at the ERDC MSRC in Year 5:

- CFD: Computational Fluid Dynamics - *ERC (Mississippi State)*

- CSM: Computational Structural Mechanics - *TICAM (Texas) and*
  ERC (Mississippi State)

- CWO: Climate/Weather/Ocean Modeling - *Ohio State*
- EQM: Environmental Quality Modeling - *TICAM (Texas)*
- FMS: Forces Modeling and Simulation/C4I - *Syracuse*

as was each of the technical infrastructure support areas:

- Scalable Parallel Programming Tools - *Rice/Tennessee*
- Scientific Visualization - *NCSA (Illinois)*
- Collaboration/Communication – *Florida State*

Mississippi State, Texas, Ohio State and Rice maintain on-site university personnel at the ERDC MSRC in support of CFD (Dr. Nathan Prewitt - MSU), CSM (Dr. Rick Weed - MSU), EQM (Dr. Phu Luong - Texas) and Scalable Parallel Programming Tools (Dr. Clay Breshears – Rice, who left in mid-year, followed by Dr. Richard Hanson), CWO (Dr. Steve Wornom - Ohio State). CSC also has a Training Coordinator on-site (Kelly Lanier-CSC).

Since the great majority of users of the ERDC MSRC are off-site, the PET effort at the ERDC MSRC places emphasis on outreach to remote users through visits to major remote user sites, training courses at such remote sites, web-based remote training delivery, and remote communication via e-mail and the ERDC MSRC PET website. Central to this outreach to all users is an ERDC MSRC User Taxonomy that has been prepared and is maintained by the ERDC MSRC PET team in order to understand the user distribution and needs. During Year 5, the ERDC MSRC PET team was in direct contact with 79 ERDC MSRC users at seventeen sites. The ERDC MSRC PET team had 82 person-days in contact with MSRC users at the annual DoD HPCMP Users Group Conference. In addition to the permanent on-site component of the ERDC MSRC PET team, other members from the team universities accumulated 157 of person-days on-site at ERDC MSRC.

Training is the most visible part of the PET program for many of the ERDC MSRC users. During Year 5, a total of 21 training courses was conducted, one of which was at a remote user site. The Training and Education Facility (TEF) at ERDC MSRC is furnished with professional quality video production and recording equipment. Training material from any source (laptop, workstation, transparencies, etc.) can be projected onto the classroom screen for instruction, broadcast over Web, and saved on videotape. Information on training courses is posted on the ERDC MSRC PET Web site:

http://www.wes.hpc.mil/

During Year 5, JSU and Florida State University continued to present distance education courses over the Web. FSU delivered one graduate course (Computational Science for Simulation Applications) to JSU and other sites, including Morgan State, NAVO MSRC, NRL, Mississippi State, and the ERDC MSRC. This offering was a full-semester, for-credit course delivered over the Web using the Tango collaborative software environment.

The enhancement of the programming environment at ERDC MSRC through the identification and introduction of programming tools, computational tools, visualization tools, and collaboration/information tools is a major emphasis of the ERDC MSRC PET effort. Twelve such tools were introduced into ERDC MSRC, or updated, by the PET team during Year 5. Training courses at ERDC MSRC and at remote user sites for many of these tools were provided, along with continual guidance and assistance in their use through the on-site team at ERDC MSRC. Other tools introduced earlier are continually supported. The ERDC MSRC PET team conducted 19 specific focused efforts during Year 5 in connection with this effort to evaluate, implement, and enhance such tools for introduction into the ERDC MSRC.

Assistance in migration of codes to the T3E, SP, and O2K was provided to ERDC MSRC users by the PET team both directly and by providing tools and technology to the ERDC MSRC Computational Migration Group at ERDC MSRC. The PET team also worked with ERDC MSRC users to enhance algorithms, physics, and visualization in user codes in the CTA areas supported at ERDC MSRC, with specific impact to 21 ERDC MSRC user codes during Year 5.

During Year 5, the ERDC MSRC PET team included 99 people from 11 universities, 38 of whom are PhDs. There were 27 person-days of travel to remote user sites, and 36 person-days at HBCUs. There were also 90 person-days of travel to national meetings for presentations related to the ERDC MSRC PET effort, to meet ERDC MSRC users, and to track technology developments in the interest of the ERDC MSRC PET effort.

A total of 21 training courses covering 39 days, were conducted on-site at ERDC MSRC, and one course covering four days was conducted at a remote user site. These on-site training courses were attended by 188 people, and the off-site course was attended by eight. A summer institute was conducted at Jackson State, impacting students from nine HBCUs. Three seminars were conducted at Jackson State, Clark Atlanta, and Morgan State. Three regular semester courses were conducted at Jackson State, Clark Atlanta, and Morgan State over the Web. The ERDC MSRC PET team produced 30 ERDC MSRC/PET technical reports, 50 conference presentations, six book chapters, and 16 journal papers reporting on efforts of Year 5.

1. Introduction

1.1 The DoD High Performance Computing (HPC) Modernization Program (HPCMP)

The Department of Defense (DoD) High Performance Computing (HPC) Modernization Program (HPCMP) was instituted in 1994 to modernize the total high performance computational capability of the military research, development, test, and evaluation (RDT&E) community to a level comparable to that available in the foremost civilian and other government agency RDT&E communities. A key component of this initiative is the DoD Major Shared Resource Centers (MSRCs).

The MSRCs provide complete HPC environments and include various types of computing systems, scientific visualization capabilities, extensive peripheral and archival storage, and expertise in use of these systems. The MSRCs support the wide variety of research and development problems arising from the science and technology programs supporting DoD's weapons development and warfighting support systems. The MSRCs provide the computer and computational sciences expertise to allow all of the DoD laboratories to advance their capability in science and technology. The types of computer systems in the MSRCs are determined by user requirements and differ from one MSRC to another.

The HPCMP selected four DoD sites to become MSRCs:

- Army Engineer Research and Development Center (ERDC), Vicksburg, MS
- Army Research Laboratory (ARL), Aberdeen Proving Ground, MD
- Naval Oceanographic Office (NAVO), Stennis Space Center, MS
- Air Force Aeronautical Systems Center (ASC), Wright-Patterson AFB, OH

In addition, DoD has identified 10 Computational Technology Areas (CTAs) as being critical across all of DoD. These 10 CTAs supported by the HPCMP are:

- CFD: Computational Fluid Dynamics
- CSM: Computational Structural Mechanics
- CCM: Computational Chemistry and Materials Science
- CEA: Computational Electromagnetics and Acoustics

- CWO: Climate/Weather/Ocean Modeling
- SIP: Signal/Image Processing
- FMS: Forces Modeling and Simulation/C4I
- EQM: Environmental Quality Modeling
- CEN: Computational Electronics and Nano-Electronics
- IMT: Integrated Modeling and Testing

An integral part of the DoD HPCMP is the provision of Programming Environment and Training (PET) at each of the MSRCs by university/industry teams in order to enable DoD researchers to develop and utilize the necessary HPC software. The PET program includes training courses in all aspects of HPC in the Computational Technology Areas (CTAs) and in relevant programming and technical infrastructure areas. It includes side-by-side transitioning of research codes into the MSRCs, as well as collaboration with MSRC users to advance and improve these codes.

The DoD HPCMP and the MSRCs are described more fully at the HPCMO Web site:

http://www.hpcmo.hpc.mil/

1.2 The Programming Environment and Training (PET) Program

The Programming Environment and Training (PET) component of the DoD HPC MSRCs is a bold and innovative approach to enhancing the capability of the MSRC users commensurate with the enhancement of the power of the hardware in the MSRCs, in order to realize the of the DoD HPC Modernization Program to attain a level comparable to that in the foremost university, industry, and other government agency HPC centers. The PET effort provides the essential user support and mode of capability enhancement necessary for the MSRCs to attain this goal - and to address the wide variety of research and development demands arising from the science and technology programs supporting DoD's weapons development and warfighting support systems.

The purpose of the PET component of the MSRCs is to enhance the entire programming environment for the MSRC users through training and support for software enhancement, addressing both near-term improvements and long-term expansions. This enables use of the MSRC computing resources to fullest capacity and extends the range of applicability of HPC to DoD technical problems.

The PET component of the MSRC program is a truly intellectual enterprise that breaks new ground in collaborative effort between DoD and academia. It establishes a two-way conduit of information and expertise to enhance the capability of the MSRC user and bring demands of DoD HPC to bear early-on in programming environment developments in progress in the universities. The PET effort is unprecedented in its concept and vision, in its management for long-term achievement, in its strong university commitment, in its approach through unique university/DoD collaboration, in its understanding and relationship between university researchers and MSRC users, and in its challenge posed in the interest of DoD to the universities and companies involved the MSRC users, and the program management.

The PET team at the ERDC MSRC has now completed its fifth year of effort. The approach of this report is to collect complete data and item lists on all aspects of the Year 5 PET effort of the ERDC MSRC into a series of tables, so that the text can concentrate on a narrative of the operation and accomplishments of the effort. More complete and continually updated information on the current PET effort of the ERDC MSRC is accessible on the ERDC MSRC PET Web site, which is accessible from the ERDC MSRC Web site:

http://www.wes.hpc.mil/

After discussing the strategic plan for the ERDC MSRC PET effort and its general implementation in Sections 2 and 3, the specific organization of the ERDC MSRC PET support structure is described in Section 4. Major accomplishments of the PET effort at ERDC MSRC during Year 5 are presented in Section 5. Of particular impact are the tools introduced into the ERDC MSRC covered in Section 6. Further specific discussion of support of ERDC MSRC users appears in Section 7. The training component of the ERDC MSRC PET effort is a major means of transferring technology to ERDC MSRC users, and this component is reported in Section 8. The HBCU/MI (MSI) element of the ERDC MSRC PET effort in Section 9 is especially important because it enhances the capability of HBCU/MIs in high performance computing and in the ability of these institutions to produce future researchers in this area. Finally, a complete list of publications arising from the PET effort at the ERDC MSRC is included in Section 10.

2. ERDC MSRC PET Strategic Plan

The strategic plan of the ERDC MSRC PET effort has evolved over the five years of operation, through close collaboration of the university team leadership with Computer Sciences Corporation and the ERDC MSRC.

2.1 Goals and Objectives

The goal of the PET effort at the ERDC MSRC is to bring university HPC knowledge and skills to bear on both the overall theme, scalable HPC applications and performance, and the specific subareas applicable to the ERDC MSRC - scalable computing migration, HPC training and DoD user productivity, HPC performance metrics/tools, management and interpretation of large data sets, SciVis for very large problems, and DoD challenge applications.

The key objectives of the PET effort in the ERDC MSRC are as follows:

- Establish a mechanism for identifying and transferring emerging advances in programming environments, computational tools, algorithms, and computational solution techniques for CTA applications from academia and industry into the ERDC MSRC.

- Create a virtual extension of the ERDC MSRC into academia that will be responsible for identifying and acquiring near-term programming environment improvements and long-term expansions, anticipating ERDC MSRC user needs and making users aware of pertinent emerging technology.

- Utilize state-of-the-art HPC technology as an inherent part of the implementation of the ERDC MSRC PET Program itself.

- Establish a training program to ensure ERDC MSRC user proficiency with transferred advances in HPC tools and technology.

- Establish cooperative development and training programs with HBCUs/MIs to significantly enhance participation in the HPC community.

- Establish effective collaboration with academia to encourage the development of graduate and Post-Doctorate programs that will enhance the skill levels and efficiency of the DoD HPC community.

Based on this, the vision for PET at ERDC MSRC is to:

- Transfer cutting edge, innovative HPC technology and tools from premier university centers to ERDC MSRC users and laboratories.

- Provide innovative collaborative environments for HPC research to all ERDC MSRC users ("remove importance of place").

- Train ERDC MSRC users in state-of-the-art HPC and scalable parallel processing (SPP) programming tools and techniques.

- Use HBCU/MI partners in an integral way to support PET objectives, enhance faculty, and train minority students in HPC.

- Enable ERDC MSRC to make major productivity gains from current/planned hardware acquisitions in PL1/2/3.

The true deliverable of the ERDC MSRC PET effort is the raised level of ERDC MSRC user capability and programming environment in the ERDC MSRC to a level not unsurpassed by academic, industry, or other government HPC centers.

2.2 Approach

The approach to PET at the ERDC MSRC is to marshal an elite and readily accessible university team to constitute a virtual extension of the ERDC MSRC into top academic expertise. This team would be able to both respond and anticipate the needs of the ERDC MSRC users for training and assistive collaboration in advancing the programming environment, utilizing a combination of strong on-site presence and dedicated support from the universities.

Support for ERDC MSRC users is provided by the PET team in the five Computational Technology Areas (CTAs) for which the ERDC MSRC is responsible:

- CFD: Computational Fluid Dynamics

- CSM: Computational Structural Mechanics

- CWO: Climate/Weather/Ocean Modeling

- EQM: Environmental Quality Modeling

- FMS: Forces Modeling and Simulation/C4I

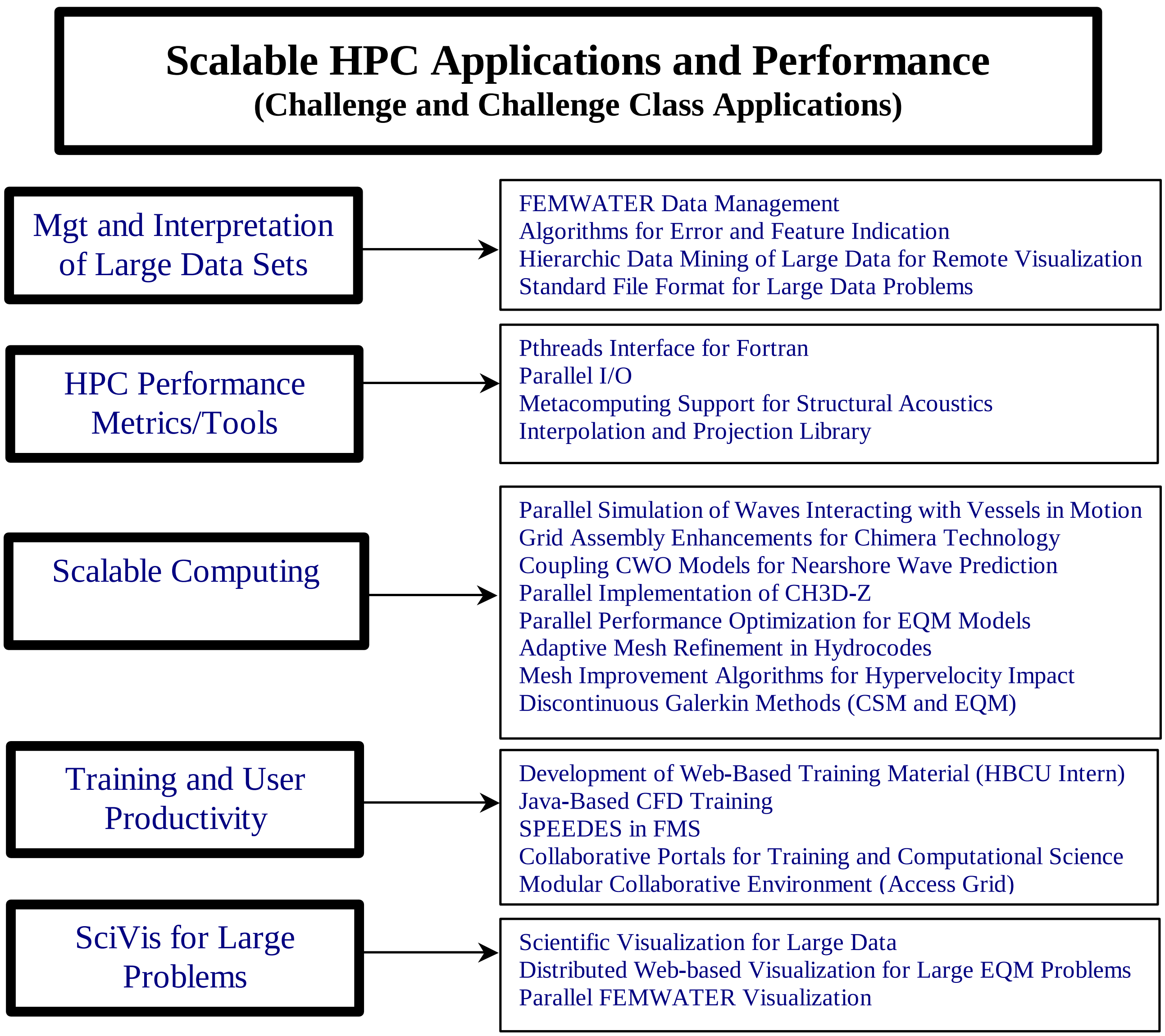
and also for three relevant technical infrastructure areas:

- Scalable Parallel Programming Tools

- Scientific Visualization
- Collaboration/Communication

The PET effort at ERDC MSRC consists of three fundamental elements: Core Support, Focused Efforts, and Training. Intertwined with these efforts are outreach to ERDC MSRC users and a program to enhance the involvement of HBCU/MIs in HPC.

ERDC MSRC Thematic Areas



Core Support provides continual interaction and assistive collaboration with ERDC MSRC users in the technical areas supported at the ERDC MSRC to migrate and enhance important codes to scalable parallel platforms and to extend the applicability of such codes and systems.

Focused Efforts address current specific projects to enhance the programming environment at the ERDC MSRC and the capabilities of ERDC MSRC users.

Training provides instruction for MSRC users, both on-site at ERDC MSRC and remote, in the technical areas supported at the ERDC MSRC and consists of both in-person and Web-based courses.

2.3 Core Support

Core Support is provided to the ERDC MSRC through continual interaction in each of five CTAs supported at the ERDC MSRC, as well as in the three technical support areas, with a specific supporting university on the PET team having responsibility for each area.

This Core Support operates primarily on-site at the ERDC MSRC, coupled with continual support from specific individuals at the university, through continual interaction and assistive collaboration of the PET team with ERDC MSRC users in the five CTAs supported at the ERDC MSRC, and in the three technical support areas, to migrate important codes to scalable parallel platforms and to enhance and extend the applicability of such codes and systems. In the operation of this Core Support, ERDC MSRC user demographics and software usage are continually monitored to provide input for identification of codes and systems of important impact.

2.4 Focused Efforts

In addition to this continual Core Support, certain specific Focused Efforts within the scope of the ERDC MSRC and the resources of the PET effort are identified for implementation by the ERDC MSRC PET team, operating across the universities when necessary. Such projects have specific objectives and deliverables. When appropriate, projects involve coordinated efforts among PET teams from other MSRCs and/or funding from other MSRC PET efforts. Interest by ERDC MSRC users in collaborative effort in such projects is a necessary factor in identification of such Focused Efforts for implementation.

2.5 Training

Training is conducted with emphasis on intermediate and advanced topics, and is coordinated across the MSRCs to reach the entire DoD user community. A state-of-the-art training facility is maintained at the ERDC MSRC with workstations for hands-on training and facilities for remote transmission. Delivery is on-site at the ERDC MSRC, in-person at some other DoD sites and at the universities as appropriate, and remotely using emerging distance learning approaches. Training specifically addresses the need to reach a growing number of DoD users, leveraging emerging digital infrastructures and the unique educational expertise of the ERDC MSRC PET team. Delivery is ultimately to be any time, any place, and at any pace.

2.6 Outreach

Since the great majority of users of the ERDC MSRC are off-site, the PET effort at the ERDC MSRC places emphasis on outreach to remote users through visits to major remote user sites, training courses at such remote sites, Web-based remote training delivery, and remote communication via e-mail and the ERDC MSRC PET Web site. Emphasis is also placed on the implementation of appropriate tools for remote collaboration, especially with regard to scientific visualization. Continually updated user demographics are assembled into an ERDC MSRC user taxonomy to guide this outreach to all users of the ERDC MSRC.

2.7 HBCU/MI (MSI) Program

The principal purpose of the HBCU/MI component of the PET effort at the ERDC MSRC is to enhance the capability of the HBCU/MI members of the ERDC MSRC PET academic team to participate fully in the PET support effort of the ERDC MSRC. To this end, ERDC MSRC PET HBCU/MIs are involved directly in Focused Efforts. Particular emphasis is placed on enhancing the opportunities of students at the HBCU/MI PET partners through Web-based university classes at the HBCU/MIs from the other PET team members and through summer institutes at the HBCU/MIs.

3. Implementation

3.1 Management

The ERDC MSRC PET effort is administered by the integrator, Computer Sciences Corporation (CSC), for the ERDC MSRC as a part of the ERDC MSRC contract. Dr. Henry Gabb of CSC was the PET Director for part of Year 5, followed by John West. Dr. Joe Thompson of Mississippi State University is ERDC MSRC PET academic team leader. Dr. Wayne Mastin of CSC, also a professor emeritus at Mississippi State, is the on-site PET team leader. Dr. Willie Brown of Jackson State University is the HBCU/MI leader. Dr. Louis Turcotte of the ERDC MSRC exercised oversight of the ERDC MSRC PET effort for the government for part of Year 5, followed by Bob Athow.

3.2 Organization

The fundamental mode of operation for PET at the ERDC MSRC is a direct and continual connection between the ERDC MSRC users and the ERDC MSRC PET team universities in support of the five Computational Technology Areas (CTAs) supported at the ERDC MSRC and three related technical infrastructure areas. This is accomplished through a combination of full-time university and CSC personnel on-site at the ERDC MSRC, in close communication with completely dedicated university personnel dividing time between the ERDC MSRC and the university, and faculty members at the university with partial commitment to the ERDC MSRC PET effort for support and leadership.

3.3 Team Composition

The university PET team for the ERDC MSRC is led by the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University, with Jackson State University as the lead HBCU/MI. The university team is as follows:

- Center for Computational Field Simulation
  (*NSF Engineering Research Center at Mississippi State*)

- National Center for Supercomputing Applications - NCSA
  (*NSF PACI Center at Illinois*)

- Ohio State University and Ohio Supercomputer Center - OSC
  (*at Ohio State*)

- Texas Institute for Computational and Applied Mathematics - TICAM
  (*at Texas*)

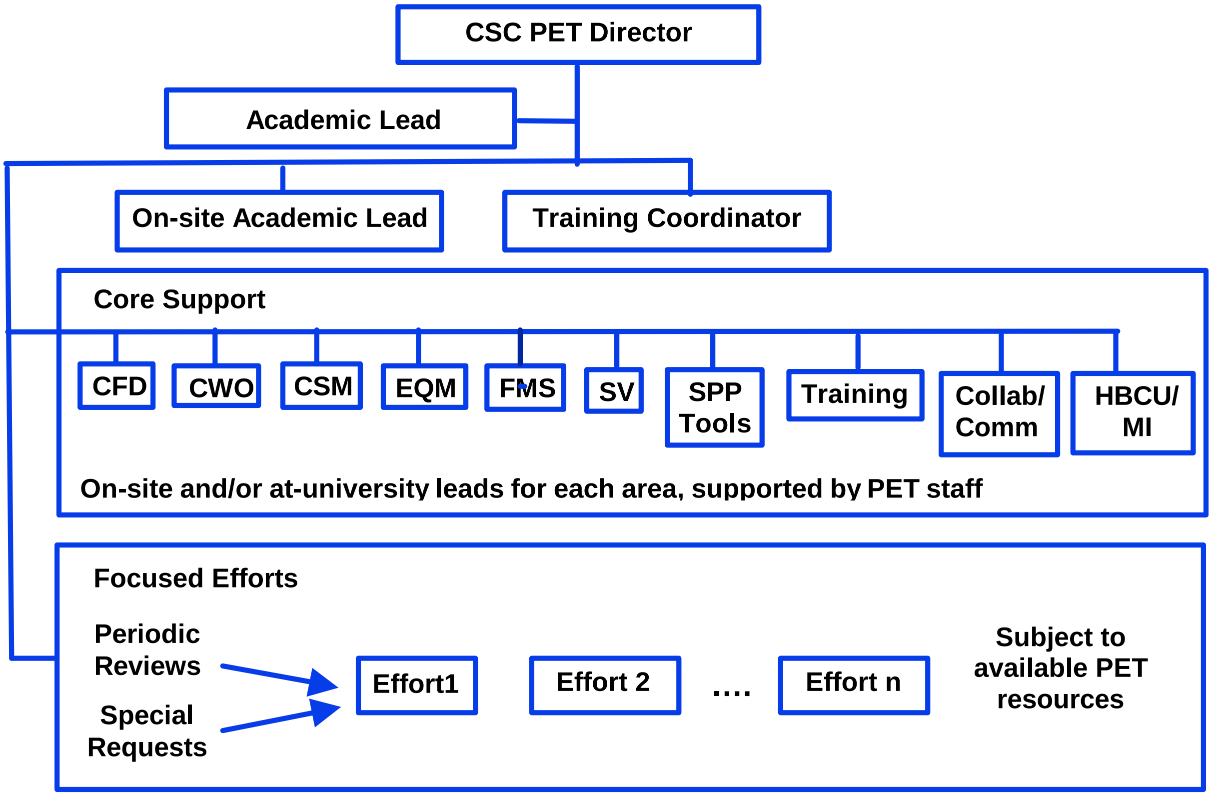
- Syracuse University
- Florida State University
- Rice University
- University of Tennessee
- University of Texas at Arlington
- HBCU/MIs: Jackson State University, Clark Atlanta University, and Texas A&M University-Kingsville

Dedicated on-site/at-university support teams for each of the five DoD Computational Technology Areas (CTAs) supported at the ERDC MSRC were the responsibility of specific universities on the PET team at the ERDC MSRC in Year 5:

- CFD: Computational Fluid Dynamics - *ERC (Mississippi State)*
- CSM: Computational Structural Mechanics - *TICAM (Texas) and ERC (Mississippi State)*
- CWO: Climate/Weather/Ocean Modeling - *Ohio State*
- EQM: Environmental Quality Modeling - *TICAM (Texas)*
- FMS: Forces Modeling and Simulation/C4I - *NPAC (Syracuse)*

as was each of the technical infrastructure support areas:

- Scalable Parallel Programming Tools - *Rice/Tennessee*
- Scientific Visualization - *NCSA (Illinois)*
- Collaboration/Communication – *Florida State*



PET Organizational Structure

Mississippi State, Texas, Ohio State, and Rice maintain on-site university personnel at the ERDC MSRC in support of CFD (Dr. Nathan Prewitt - MSU), CSM (Dr. Rick Weed - MSU), EQM (Dr. Phu Luong - Texas), CWO (Dr. Stephen Wornom - Ohio State) and Scalable Parallel Programming Tools (Dr. Clay Breshears – Rice, who left in mid-year). CSC also has a Training Coordinator (Kelly Lanier - CSC) on-site.

3.4 Reporting and Technology Transfer

Transfer of emerging technology from the academic community into the ERDC MSRC is a primary purpose of the ERDC MSRC PET effort. Also important is transfer in the other direction, providing input and feedback regarding emerging DoD needs to influence developments at universities. The primary mode of technology transfer in the ERDC MSRC PET effort is direct contact between the PET team and the ERDC MSRC users. The PET team also produces a series of reports on technology developments for distribution to ERDC MSRC users, and technology transfer is a prime emphasis of the training component of the ERDC MSRC PET effort. The on-site personnel at the ERDC MSRC from the PET team form a continual conduit for technology transfer.

4. Technical Support Teams

The fundamental mode of operation for the PET support effort at the ERDC MSRC is a direct and continual connection between the ERDC MSRC PET team universities and the ERDC MSRC users in support of the five Computational Technology Areas (CTAs) supported at the ERDC MSRC and three related technical infrastructure areas.

This is accomplished through on-site PET team members at the ERDC MSRC in close communication with PET team members at the supporting universities who also make frequent visits to ERDC MSRC. The PET team members on-site at ERDC MSRC are full-time university personnel, supplemented by CSC personnel. The on-site PET team members at the ERDC MSRC are key to the ERDC MSRC PET operation, since these team members are the front line of contact with ERDC MSRC users.

These six on-site team members during Year 5 were:

- Lead: Dr. Wayne Mastin - CSC (Professor Emeritus, Mississippi State)
- CFD: Dr. Nathan Prewitt - Mississippi State
- CSM: Dr. Rick Weed - Mississippi State
- CWO: Dr. Steve Wornom - Ohio State
- EQM: Dr. Phu Luong - Texas
- SPPT: Dr. Clay Breshears – Rice (left in mid-year, followed by Richard Hanson)

Also on-site at ERDC MSRC were the overall PET Project Leader, Dr. Henry Gabb part of the year followed by John West, and the Training Coordinator, Kelly Lanier, all of CSC.

A complete listing of all the ERDC MSRC PET team personnel is given in Table 1. During Year 5, the eight technical support teams in the ERDC MSRC PET effort operated as follows:

4.1 CFD: Computational Fluid Dynamics CTA

(ERC - Mississippi State)

As part of the PET effort at the ERDC MSRC, CFD support is the responsibility of the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University. The University CFD Lead is Dr. Bharat Soni and the On-Site CFD Lead is Dr. Nathan Prewitt. The On-Site CFD Lead (Prewitt) serves as an effective administrative liaison between the ERDC MSRC, CSC, and MSU, and as a technical liaison among ERDC MSRC users and the entire CFD support team. The On-Site Lead also coordinates communication and facilitates interaction with other components of the ERDC MSRC PET team. This includes maintenance of the CFD Web page content and regular activity reporting.

The CFD team in the ERDC MSRC PET effort serves the ERDC MSRC by providing program-wide CFD support, R&D expertise on selected technology enhancements, and HPC assistance for targeted codes. Program-wide support includes direct ERDC MSRC user contact and community cultivation, technology transfer, outreach, participation in workshops and technical meetings, user training in HPC, and other duties. HPC support for targeted codes and delivery of collaborative R&D expertise were more specific tasks selected to provide technology that has potential application and interest throughout the ERDC MSRC user community.

Along with core support activities including training, technology transfer, outreach and CFD parallel software enhancements, Bharat Soni and Nathan Prewitt have led focused efforts on Chimera Grid Assembly, the development of INLiB: Interpolation Library - in collaboration with CSM (Graham Carey) and EQM (Mary Wheeler) of the University of Texas at Austin, and the development of CFD Learning Tool. MSU researchers Roy Koomullil, Sankarappan Gopalsamy, and David Thompson have also contributed to these focused effort projects.

4.2 CSM: Computational Structural Mechanics CTA

(TICAM – Texas, with ERC – Mississippi State)

The technical support team members for CSM include Drs. J.T. Oden, Graham Carey, David Littlefield, Robert McLay, Atanas Pehlivanov, and Serge Prudhomme. J.T. Oden and Graham Carey serve as University CSM Co-Leads. David Littlefield was the primary technical contributor to the focused effort concerned with adaptive mesh refinement and CTH capability and algorithm enhancements. Robert McLay contributed to the focused effort dealing with adaptive mesh technology, mesh improvement and algorithms for hypervelocity impact and penetration analyses. Atanas Pehlivanov worked on the Hierarchical Data Mining focused effort. Serge Prudhomme contributed to the focused effort concerned with discontinuous Galerkin finite elements and adaptive grids for DoD problems.

Dr. Rick Weed (Mississippi State) serves as the On-Site CSM Lead at the ERDC MSRC. As On-Site Lead, Dr. Weed's duties encompass a wide range of direct support activities for ERDC MSRC users. These duties include conducting training classes in parallel programming methods, programming support for on-going HPCMP Challenge projects and CHSSI code projects, and programming support for TICAM core support and focused effort activities.

4.3 CWO: Climate/Weather/Ocean Modeling CTA

(Ohio State)

The University CWO Lead for the Ohio State CWO PET team is Dr. Keith Bedford. Dr. Bedford is Chair of the Department of Civil and Environmental Engineering and Geodetic Science (CEEGS). The CWO Academic Co-Lead is Dr. Ponnuswamy Sadayappan, Professor of Computer and Information Science. Additional team members are Dr. Stephen Wornom (CEEGS), the On-Site CWO Lead, and Dr. David Welsh (CEEGS), a university-based research scientist.

Drs. Bedford and Sadayappan provide management-level project guidance as well as technical input and review in their own areas of expertise. They are responsible for overall project coordination, contacts with government and integrator management, identification of strategic goals, monitoring of progress toward project deliverables, and financial and contract management. Dr. Bedford is closely involved with technical matters concerning CWO physics and numerical modeling strategies, while Dr. Sadayappan takes the leading role on issues of code optimization, parallelization, and migration.

Dr. Wornom's chief roles are to offer ongoing, responsive support to on- and off-site ERDC MSRC users in the CWO and related fields, and to act as a facilitator for interaction between those users and the university-based team members. To this end, Dr. Wornom maintains frequent contact with CWO users. These contacts include general goal-setting discussions, collaborative improvement of code physics, software evaluation and code-enhancement related to high performance computing (HPC) techniques, and knowledge transfer by means of training workshops.

Dr. Welsh's main focus is on the upgrade of CWO numerical model physics, with a particular emphasis on model coupling. Within this area, Dr. Welsh takes the technical lead on focused effort activities, while offering backup to Dr. Wornom on core support activities. In his focused effort work, Dr. Welsh also addresses model performance using established HPC tools. Dr. Welsh takes a leading role in the initial development of reports, presentations, and proposals and is a significant contributor to training workshop materials.

4.4 EQM: Environmental Quality Modeling CTA

(TICAM – Texas)

The PET team for EQM includes Drs. Mary F. Wheeler (University EQM Lead), Clint Dawson, Phu Luong (On-Site EQM Lead), Victor Parr, Eleanor White Jenkins, and Krzysztof Banas. Wheeler and Dawson provide technical leadership and assistance in numerical analysis and computational science as well as teach tutorials and conduct workshops. Luong's efforts were devoted to organizing training classes, making contacts with ERDC MSRC EQM users, organizing workshops in conjunction with UT personnel, and working on specific codes with ERDC EQM users and NAVO EQM users. Wheeler, Dawson, and Luong were also involved in collaborations in developing conference posters, conference papers, and journal papers. Parr's activities centered on parallelization, debugging, validation, and evaluation of several EQM codes as well as working with Jenkins on the grid projection code development. Banas developed discontinuous Galerkin methods for water quality modeling.

4.5 FMS: Forces Modeling and Simulation/C4I CTA

(Syracuse)

The Year 5 PET FMS was a single person effort, conducted by Dr. Wojtek Furmanski at Syracuse University as a continuation and completion of the larger ERDC MSRC PET FMS effort pursued by NPAC in previous years.

4.6 C/C: Collaboration and Communication

(Florida State, earlier Syracuse)

The training, collaboration and communication efforts led by University C/C Lead Dr. Geoffrey Fox consisted of two distinct phases in Year 5. From April 2000 to mid-May 2000, all the personnel except Fox were situated at and paid by Syracuse University. From mid-May 2000 onwards, all the personnel working on the effort on an ongoing basis moved to Florida State University and were paid by FSU. There was a transition period through the end of June 2000 when personnel were paid by Syracuse. The key person in this transition was Dr. David Bernholdt, who was essential in ensuring a smooth transition. Bernholdt now works at Oak Ridge National Laboratory. The team at FSU consists of Fox and several Ph.D. students working in portal, collaboration, and Internet technology areas.

4.7 SPP Tools: Scalable Parallel Programming Tools

(Rice and Tennessee)

4.7.1 Rice

The Rice SPPT team consisted of two computing professionals, Drs. Clay Breshears(On-Site SPPT Lead) and Richard Hanson (University SPPT Co-Lead). Dr. Breshears left in mid-year, after which Hanson spent half-time at ERDC MSRC assuming the role as On-Site Lead.

4.7.2 Tennessee

The Tennessee (UTK) SPPT PET team consists of staff members of the Innovative Computing Laboratory (ICL) led by Dr. Jack Dongarra. ICL has been a leader in producing high performance computing software and tools for more than a decade. Dr.

Shirley Moore (formerly Browne) coordinates the overall UTK PET Scalable Parallel Programming (SPP) Tools effort as University SPPT Co-Lead, and worked on projects. Other UTK staff who worked on Year 5 projects included Dr. Graham Fagg, Dr. David Cronk, and Dorian Arnold.

4.8 Scientific Visualization

(NCSA – Illinois)

The NCSA Scientific Visualization PET team has Dr. Polly Baker as University SV Lead. Dr. Alan Shih served as project lead for the focused effort on "Visualization Tools for EQM." Dr. Mike Folk was project lead for the focused effort "Standard File Format for Large Data Problems and Visualization." Muqun Kent Yang also worked on the file format project.

5. Year 5 Accomplishments

As noted above, the PET effort at the ERDC MSRC operates by providing core support to ERDC MSRC users, performing specific focused efforts designed to introduce new tools and computational technology into the ERDC MSRC, conducting training courses and workshops for ERDC MSRC users, and operating an HBCU/MI (MSI) enhancement program.

The major accomplishments of the ERDC MSRC PET effort in enhancing the programming environment at the ERDC MSRC are described in this section. The presentation is according to CTAs and technical infrastructure support areas, but many of the efforts overlap.

Tools introduced into the ERDC MSRC in the course of Year 5 of the PET effort are described in Section 6. Specific ERDC MSRC codes impacted by the PET effort during Year 5 and assistance from MSRC users with such codes and applications are described in Section 7. More detail on the Year 5 effort is given in the ERDC MSRC PET Technical Reports and other publications from Year 5 that are listed in Section 10. Training conducted during Year 5 is described in Section 8. The accomplishments in the HBCU/MI (MSI) component of the ERDC MSRC PET effort are discussed in Section 9. Finally, a list of publications and presentations related to ERDC MSRC PET during Year 5 is given in Section 10.

5.1 CFD: Computational Fluid Dynamics CTA

(ERC – Mississippi State)

PET CFD support is broken down into core support and focused effort projects. The progress realized in the core support and the three focused projects on Chimera Grid Assembly, INLiB, and CFD Learning Tool is described in this section. Three technical reports summarizing progress and technical contributions made in these projects have been submitted to ERDC MSRC for publication.

The lack of an on-site lead and focused effort funding decreased the amount of tools installed at ERDC MSRC to support CFD users. This year, great strides have been made to improve this situation. Several tools (such as PMAG, INLib, CFDtool, GridTool, GGTK, etc.) that are being completed through focused efforts, or were developed under funding that leveraged PET funding, will be installed at ERDC MSRC by June 1, 2001.

5.1.1 Core Support: Outreach, Tech-Transfer, and Training

The core support involving outreach, technology transfer, training, and technology improvements was provided as a team effort between Drs. Nathan Prewitt and Bharat Soni. Concentration was placed on validation and improvements in the CFD CHSSI software. In particular, minor bug fixes, improvements in *makefiles* and utilities were provided to Drs. Robert Meakin (U.S. Army – Aero Flightdynamics Division) and William Chan (NASA Ames).

A CFD CHSSI software session was organized at the *39th AIAA Aerospace Sciences* meeting in Reno in January. This was a joint effort among ARL, ASC and ERDC PET programs. This special session was attended by 30 DoD CFD researchers. All CHSSI CFD software developers made presentations, and Drs. Jay Boris and Bharat Soni chaired the session. The DoD CFD CTA leads, Drs. Jay Boris and Jere Matty, and Dr. Larry Davis of HPCMO made comments during the panel discussion. This session was very successful and provided an excellent opportunity to outreach and transfer CFD CHSSI software technology to the DoD community at large. Seminars representative of the current state-of-the-art and state-of-the-practice were organized. In particular, seminars on the Current State of the Cartesian Grid Based Code CART3D (Michael Aftosmis, NASA Ames), Chimera Technology (Nathan Prewitt), Grid Generation and Geometry Treatment (Bharat Soni), Unstructured Grid Based CFD Solver (Ravi Ramamurti, NRL), CFD Codes for Hydrodynamic Simulations (Bob Bernard, ERDC), Wind Generation Simulation (Paneer Selvam, University of Arkansas), and the LOCI Framework (Ed Luke, MSU) were successful with good user participation.

Dr. Soni also gave an invitation only one-hour talk on the development of the GGTK-Geometry-Grid Tool Kit at the *39th AIAA Aerospace Sciences Meeting* in Reno in January. Contributions were made to poster sessions at the *7th International Grid Generation Meeting* and the *9th International Meshing Roundtable*. A CFD Newsletter describing PET activities was published and distributed at the CFD and Grid conferences and to MSRC users. A CFD Poster was designed with pictorial views presenting highlights of successes and was displayed at all MSRC sites and at HPCMO.

Dr. Soni, with the help of MSU researchers Drs. Roy Koomullil and David Thompson, conducted part of the JSU HPC Summer Institute. The JSU Summer Institute students were provided lectures and demonstrations of HPC and CFD applications and methodologies. Two days of "hands-on" experience with the CFD application execution process and visualization software were provided at JSU. The Java-based exercises were very useful in demonstrating flow field characteristics and the importance of simulation. MSU's hybrid grid-based flow solver and grid generation software were utilized to demonstrate the simulation process to students. The visualization was very attractive the JSU Summer Institute students, who gained insight into HPC and CFD simulation processes. Following the program's success, the CFD Learning Tool developed under a focused effort project will be utilized to provide "Hands-On Experience in CFD" to JSU Summer Institute students in 2001.

5.1.2 Chimera Grid Assembly and Overset Technology Knowledge Center participation

The use of overlapping structured grids (i.e., Chimera technology) has shown an excellent potential for addressing CFD flow solutions involving geometrically complex domains and domains containing moving or deforming boundaries. For example, CFD simulations using Chimera technology have been performed for such diverse applications as cluster parachutes, helicopter aerodynamics, and store separation. These examples represent time-accurate, multidisciplinary simulations on time-dependent domains that are directly related to the DoD warfighting mission. The CHSSI codes OVERFLOW-D and WIND, the Beggar code from Eglin AFB, and the PEGSUS code from AEDC are all software packages based on Chimera technology.

One of the major obstacles to the widespread use of Chimera technology is the process of establishing communication between the overlapping structured grids. This process is referred to as the "grid assembly" process. Grid assembly includes two major processes: hole cutting and stencil searching. Hole cutting is used to blank out any points from the overlapping grids that do not lie in the solution domain. The stencil search is used to identify interpolation stencils that allow the solution from one grid to be interpolated onto another overlapping grid. This focused effort is loosely defined to improve upon the existing grid assembly data structures and algorithms.

In support of this project, Chimera researchers Robert Meakin (U.S. Army – Aero Flightdynamics Division), William Chan (NASA Ames), Robert Nichols (AEDC), Jubraj Sahu (ARL), Jim Brock (Eglin AFB), and Ralph Noack (MSU, ARL MSRC On-Site CFD Lead) were contacted to establish a collaborative relationship. This project is closely associated with the Overset Knowledge Center being organized by Ralph Noack in PET at ARL MSRC, and is leveraging related work on the Chimera Tool Kit (CTK), which is a project at MSU/ERC funded under DEPSCoR from ARO.

As part of this collaborative effort, *endian* conversion utilities and *makefile* bug fixes for the OVERGRID code were provided to William Chan. OVERGRID has also been installed at ERDC MSRC, and at the MSU/ERC for student use. Ruparani Chittineni, a graduate student at MSU/ERC, is developing a direct CAD interface for OVERGRID. *makefile* improvements have also been made for the OVERFLOW-D code and efforts are being pursued to improve the capabilities and usability of the 6DOF routines within OVERFLOW-D. This is a requirement for the Challenge project owned by Jubraj Sahu (ARL). Contributions of presentation and reference materials have also been made to the Overset Knowledge Center at ARL MSRC, as well as participation in planning for the organization, scope, and road map for the center.

One technique being used to help improve the data structures and algorithms used in grid assembly is visualization. David O'Gwynn, a graduate student at MSU/ERC, is developing a code used to visualize the PM tree data structure used by the Beggar code. This code, tentatively called "pmdebug," allows the interactive visualization and interrogation of the octree data structure and the facets of the Binary Space Partitioning (BSP) trees that make up the PM tree. The code, which is being written in a machine portable way using Python, C/C++, OpenGL, and several alternative GUI toolkits, will allow users to analyze grid assembly problems, as well as help developers to debug problems with the data structure itself.

In collaboration with Dr. Dan Duffy (CSC/CMG), Nathan Prewitt has worked on improving the parallel performance of the grid assembly algorithms in Beggar. This work uses shared memory programming constructs to allow a fine-grain treatment of the stencil search process. In connection with dynamic load balancing, this allows for great improvements in the load balance of the grid assembly process and thus improves the scalability of the overall simulation. This work has been accepted for presentation at the *15th AIAA CFD Conference* and at the *2001 DoD HPCMP Users Group Conference*. An ERDC MSRC PET technical report has also been written to document some of this work.

5.1.3 INLiB Development

Interpolation/approximation (with desired tolerance), as well as grid manipulation and similar tools, are utilized at many DoD simulation steps. This starts with pre-processing, geometry preparation and grid generation and continues with post-processing and visualization associated with numerical simulations relevant to CFD, CSM, CWO, and other CTAs. This is becoming more important as the work increases with domain decomposition, multilevel strategies on different grids, load balancing for parallel scalable simulations, and coupled multiphysics on different grids. The accuracy of the interpolation/projection schemes and their properties (tolerance control associated with the approximation scheme, local conservation constraint satisfaction, contact restrictions, etc.) are very important to the integrity of the overall simulation process. This is especially true when dynamically moving/deforming/changing grids are utilized and when multidisciplinary applications requiring distinct grid resolution/strategies are employed. In the case of certain field simulations, conservative interpolation of physical characteristics is extremely important. Another area of growing concern and broad interest in the DoD user community is the use of approximation schemes pertinent to data screening and reduction for rapid remote visualization and interpretation of very large simulation datasets. Here, data manipulations may be based on the region(s) of interest and/or the relevance of physical features.

Various algorithms and software components to address the above issues are available in the literature and in the public domain to perform interpolation/approximation in a piece-meal fashion. Researchers are also exploring distinct interpolation/approximation algorithms within the academic/NASA/DoD community. However, there is no coherent library/toolkit accessible to the DoD community to provide these functions. In response to this need, the development of the INLiB (Interpolation Library) was initiated as a collaborative PET effort between MSU and the University of Texas at Austin.

An alpha version of INLiB – interpolation, approximation, and grid manipulation - has been completed. This library contains stand-alone interpolation and approximation modules applicable to multidisciplinary simulations involving CFD, CSM, CWO, and other CTAs. The toolkit modules are accessible from Fortran, C and C++ applications via APIs. The following modules have been incorporated and validated in the INLiB:

- Linear, Bilinear, Trilinear, Bezier, B-Spline, and NURBS interpolation and approximation functions;

- Interpolation/approximation of various geometric entities into NURBS representation;

- Interpolation modules used for generation of structured grids (transfinite interpolation, transformations, etc.);

- Interpolation of solution properties between distinct grid strategies/resolutions.

The development to include the following modules is under way:

- Feature detection module;

- Weighted interpolation/approximation of solution characteristics addressing conservative properties;

- Hierarchic extraction module;

- Error indicator module;

- Grid quality assessment module.

This software toolkit/library will be very useful to DoD researchers involved in numerical field simulation and Multidisciplinary Optimization research. There is a plan to release the beta version of INLiB to the DoD community at large by September 2001. A PET technical report summarizing the current progress in INLiB with mathematical details of interpolation modules has been submitted to ERDC MSRC for publication.

5.1.4 CFD Learning Tool Development

One of the missions of the MSRC PET program is to educate a new generation students and DoD practitioners in HPC and its applications in solving large-scale simulation problems. Under ARL and ASC PET, a Web-based training course in grid generation is being developed at MSU. Last year, the Web-based tool *jvwt* (Java virtual wind tunnel), which was developed at MIT, was acquired and enhanced to demonstrate CFD simulation process to undergraduate students at JSU. The development of a Web-based training and demonstration tool has been initiated. This tool will be utilized to teach and demonstrate basic concepts of CFD and HPC to students, young engineers, and non-CFD DoD practitioners. This development provides a basis for future development of Web-based training tools for CHSSI software for CFD practitioners**.** This tool is based on a graphical user interface and provides interactive visualization and control to various selections (boundary conditions, geometry, grid, flow variables to visualize, numerical schemes to exercise, dissipation order to apply, angle of attack, and contour vs. line plots, etc.). The software contains various numerical schemes, boundary conditions and macros for geometry and grid information. MSU's hybrid grid generation and flow solver are utilized in this development.

The beta version of the CFD Learning Tool has been completed and was demonstrated at the PET annual review meeting at the ERDC MSRC. Work continues on additional functionality and validation. This software will be released to the DoD CFD community at large in September 2001. A PET technical report summarizing this development has been submitted to ERDC MSRC for publication.

5.1.5 Parallel Simulation of Wave Break and Waves Interacting with Vessels in Motion

In this project, conducted by Clark Atlanta University, the CAU parallel finite element flow solver was applied to simulate breaking wave problems, investigating the structure of wave formation and wave break in a computer environment resembling the physical condition. The flow solver is also applied to simulate waves interacting with vessels in motion. This project involved extensive collaborations and discussions with Drs. Charlie Berger and Jane Smith from the ERDC CHL.

First, the 3D test problem initiated last year in PET was completed. Computations were performed for flow in a contraction channel using a much more refined mesh. The computed results compare very well with the experimental data. Second, simulations were carried out for wave formation and wave breaking characteristics. The results were discussed with Dr. Jane Smith from ERDC CHL. Based on Smith's feedback, the simulations are extremely promising. Third, one of the largest finite element applications on the 1088-processor Cray T3E-1200, located at the AHPCRC, was performed. Waves interacting with two ships traveling side by side were simulated using a finite element mesh with more than 200 million tetrahedral elements. To obtain the solution, a coupled system of equations with nearly 175 million unknowns was solved more than 1,000 times. The sustained computation speed was around 130 GigaFLOPS. In collaboration with Dr. Andrew Johnson (AHPCRC-NetworkCS), remote visualization was performed for this large application. In this approach, the need to FTP the large data sets from the Cray T3E to visualization workstations was eliminated. The most recent computations simulated the hydrodynamics of ships in motion using unstructured meshes with more than one billion elements. A paper on this work was presented at the *7th International Grid Generation Meeting* in September.

5.2 CSM: Computational Structural Mechanics CTA

(TICAM – Texas, with ERC – Mississippi State)

The principal goal of the TICAM PET CSM effort is to introduce, implement and test adaptive grid techniques for analysis of CSM problems for DoD simulation of "violent events" such as those encountered in blast and hypervelocity impact studies and the related problem of analysis of damaged structures. Also of interest are work on new algorithms and techniques related to large-scale parallel simulation of these classes of computationally intensive and complex applications. Representative DoD codes include CTH and EPIC, as well as interfacing such simulations to other analysis codes. This work requires consideration of the following:

- Appropriate *a posteriori* error estimates and corresponding indicators for these problem classes;

- Strategies for adapting the grid by refinement, coarsening, and redistributing or smoothing strategies;

- Complications in implementing the adaptive schemes related to the form of "legacy codes";

- Development and incorporation of appropriate data structures for adaptive refinement and coarsening;

- Development of indicators to assess the degradation in the quality of the elements during simulation as the grid is refined or deforms;

- Efficiency in implementation; and

- Parallel, scalable HPC needs with respect to partitioning for domain decomposition and for parallel adaptive simulation.

Core support and focused effort activities have been targeted at these goals and there has been progress in several significant areas.

5.2.1 CSM Core Support

Activities in core support over the past year have been closely coordinated with focused efforts, and have involved the organization of a number of mini-symposiums, workshops, and presentations. Dr. Carey organized a number of sessions at the *ASTC High Performance Computing Symposium*. Several papers concerning the focused efforts were also presented. At *FEF 2000*, organized in part by Drs. Oden and Carey, a number of sessions and individual papers were given as part of this effort. Dr. Oden gave a presentation in Washington in support of the PET Program, highlighting the CSM success stories and accomplishments achieved in the effort. Dr. Carey taught a short course on computational grids at the *Eighth International Meshing Roundtable*, where he was also a panel participant. In addition, there has been continued work with other researchers at ERDC and at Sandia National Laboratories in connection with the CTH AMR focused effort.

5.2.2 Adaptive Mesh Refinement (AMR) and CTH Capability and Algorithm Enhancements

CTH is a multi-material Eulerian wave propagation code developed at Sandia National Laboratories for the analysis of DoD and DoE applications involving violent events. These applications include blast damage studies of buildings such as those occurring in natural disasters or in terrorist attacks and other applications such as hypervelocity impact of penetrators. CTH is a very large hydrocode that includes very complex multi- material constitutive models and is widely used in DoD applications studies. The code is based on explicit integration of the underlying conservation equations using hexahedral elements. It can be viewed as an established legacy code for which development can be measured in excess of many tens of man-years. The code was initially developed for serial and vector processing on previous generation architectures using standard spatial discretization strategies. There is a strong effort under way to upgrade the capability of CTH and similar codes to provide more reliable and efficient scalable efficient solutions. The focus of the present work has been directed to this goal by technology transfer of ideas that have been demonstrated in the research community on simpler problem classes and that deal with parallel Adaptive Mesh Refinement (AMR) techniques.

There has been collaboration with D. Crawford (Sandia) to introduce both parallel-distributed analysis capability with AMR into CTH. The AMR technique is based on a 2:1 block refinement approach with no two adjacent blocks more than one level apart in the associated refinement tree. The problem is complicated by the need to treat the multi-material behavior appropriately. The code is operational in parallel. The production code will be released to ERDC Structures Lab shortly. An operational research version of the code has already been installed at the ERDC MSRC and is nearing readiness to perform production-level computations. The research version contains several enhancements that will not be immediately available in the production version. This includes an Eulerian model for incorporation of rigid barriers of arbitrary shape, and an interface to allow direct extraction of pressure data for generation of load curves. The latter enhancement has been designed to interface with the INGRID software package to permit coupling of CTH pressure data with DYNA structural calculations.

CTH is a major analysis code used for simulation of explosive events by the DoD community. The new work and associated upgrade will permit more reliable, efficient analysis of this class of problems. In turn, this implies that many time-critical simulations will now be possible where before they could not have been reliably computed in time.

5.2.3 Adaptive Mesh Technology, Mesh Improvement and Algorithms for Hypervelocity Impact and Penetration Analysis

In this focused effort, the development and implementation of error indicators for adaptive grids arising in, e.g., Eulerian and Lagrangian impact and penetrator calculations of interest to the DoD community. As a representative example of a Lagrangian code, consider the elasto-plastic impact code (EPIC) developed by G. Johnson at Alliant systems. There are similar ideas for the Eulerian code CTH described in the previous focused effort. The Lagrangian code calculation is further complicated by the deformation of the elements in the grid, so element shape quality may deteriorate locally and degrade both accuracy and efficiency. The question of dynamic partitioning of the associated unstructured grids that arise through the adaptive process has been addressed.

The capability of EPIC has been expanded to permit local adaptation of the grid by edge bisection and point insertion in concert with coarsening of the grid through element removal. Several new error indicators have been added and supporting analysis has been developed. The Taylor "anvil" benchmark is the basic test case. Metrics were developed to assess the shape quality of the deforming elements, and new residual indicators are being investigated for the Eulerian code class.

As the analysis simulations become larger and more complex, the validity and reliability of the results may be suspect. The indicators on error and element shape quality provide a mechanism for assessing and maintaining reliability of the simulations and enhancing efficiency. This work is broadly applicable to other DoD simulators. The adaptive strategy for the Lagrangian application code EPIC has demonstrated that one can extend the effective time period of computation by an order of magnitude, and suggests this can be further improved since EPIC simulations can fail due to diminishing timesteps as the mesh degrades.

5.2.4 Discontinuous Galerkin Finite Elements and Adaptive Grids for DoD Problems

The purpose of this effort is the development, analysis, testing, and implementation of discontinuous Galerkin finite element methods (DGM) for finite element simulations. Such methods are of growing interest for certain finite element applications in the research community. They appear particularly appealing for transient simulations of applications with shock-like structures and similar hyperbolic or near hyperbolic problems of interest to DoD users. In the DGM schemes, the continuity requirements across the interfaces between elements are enforced only weakly in the variational formulation rather than in the basis itself. This implies that the degrees of freedom can be local to the element level, with easier migration to higher degree elements. Stability and other properties may also be improved relative to other more conventional formulations.

One particular area of interest is the development and testing of *a posteriori* error estimates to assess the accuracy of the approximations and to design an adaptive grid methodology in order to control numerical errors. There has been a renewed interest in DGM recently, primarily due to the discovery that variants of these methods could be used effectively to solve diffusion problems as well as problems of pure convection.

Work has focused so far on *a priori* and *a posteriori* error estimation for several types of methods including the Baumann-Oden version of DGM; theoretical work on the mathematical foundation of DGM is also under way. In the case of *a priori* error estimation, optimal or near optimal rates of convergence with respect to the mesh size h and the spectral order p have been achieved. On the other hand, testing of *a posteriori* error estimator is based on the residual of the partial differential equation. Our first numerical results are very promising. The next step in this effort will focus on developing an adaptive strategy for structured and unstructured meshes aimed at enhancing the accuracy and performance of CSM codes.

5.2.5 Algorithms for Error and Feature Indication in Interpolation and Approximation

The TICAM members are carrying out collaborative work on algorithms and software for error or feature indicators that can be used in conjunction with the interpolation library

(INLiB) routines provided by Dr. Bharat Soni of MSU in PET. The TICAM team members will also contribute work on *h*, *p*, and *hp* approaches suitable for these classes of approximation.

The *h*-adaptive approaches are being applied in numerical tests on the "TESTBED" software being developed in support of other focused effort activity. The CSM TICAM group is also working on software for projections among different grids including constrained projections for interfaces in multi-physics applications involving different CSM codes. The proposed library will be of broad use to analysts using computational grids in the DoD community (e.g., for post-processing).

5.2.6 Hierarchic Data Mining for Very Large Scale Data Sets for Remote Visualization and Manipulation

The problem of extracting the salient features from data and manipulating it on a remote workstation is a major stumbling block. The proposed work will explore ongoing work on hierarchic adaptive strategies typical of those used in adaptive finite element algorithms, but applied here to the problem of hierarchic extraction and manipulation of data from simulations on unstructured or structured grids. A plan has been made to develop and test the idea on very large-scale simulation results arising in PET focused effort studies in support of ERDC MSRC. This work is of interest to CSM and other DoD applications groups where similar difficulties and needs arise in interrogation and rapid remote display of hierarchically screened datasets (e.g., the project of S. Aliabadi of Clark Atlanta University in PET).

The purpose of this project is to promote and develop large-scale data mining that will enhance the capability and utilization of codes used by DoD researchers. This is a pervasive problem in many areas of interest to DoD including CSM, CFD, and CWO. The basic problem is one bred of success – the ability to assimilate masses of data either from experiment, field work or simulation – but interpretation remains a problem.

s CWO: Climate/Weather/Ocean Modeling CTA

(Ohio State)

5.3.1 Coupling the SWAN and WAM Wave Models for Accurate Nearshore Wave Predictions

The aim of this core project conducted by CWO PET team members Stephen Wornom, David Welsh, and Keith Bedford was to investigate the benefit of nesting a shallow water wave model within a deep water wave model. The motivation was that enhanced accuracy in nearshore wave predictions aids environmental impact studies and naval operations planning. Coupled deployments of the WAM deep water model and the SWAN shallow water model were used to simulate wave activity during Hurricane Luis off the coast of North Carolina. Data from the ERDC FRF in Duck, NC, were used for evaluation of coupled and stand-alone WAM runs. Triad wave-wave interaction and depth-induced breaking are two shallow water effects included in SWAN, but not in WAM. It was found that the triad interactions had a negligible effect on SWAN predictions, but depth-induced breaking reduced the storm peak wave height by 20 percent. This resulted in coupled SWAN predictions that were indeed closer to the measured values than were the WAM predictions.

This work was carried out at the request of Dr. Bob Jensen of ERDC CHL. Dr. Jensen has a significant responsibility for the development of DoD operational and rapid-response wave forecasting activities. During the work, there was also frequent interaction with SWAN user Dr. Erick Rogers of NRL Stennis. One benefit of this project was an ERDC PET workshop entitled "Introduction to the SWAN Wave Model." This class was attended by 12 CWO scientists, mainly from ERDC, NRL Stennis, and NAVO.

5.3.2 Effect of the Wave Propagation Schemes on Nearshore Wave Predictions

This core project – conducted by Stephen Wornom, David Welsh, and Keith Bedford – was an outgrowth of the SWAN and WAM coupling project discussed above. Both models can be deployed using either Cartesian or spherical grids. One major difference between the two types of grids is that spherical projection accounts for the Earth's curvature, but Cartesian projection does not. For computational domains that cover a large geographical area, it would be expected that Cartesian projection would cause wave prediction errors. Conversely, as the size of the domain becomes small, only minor differences between predictions made using equivalent spherical and Cartesian grids would be expected. This project examined the magnitude of such differences using the WAM code and small nearshore grids. Based on wave observations from the ERDC FRF, Duck, NC, it was found that Hurricane Luis Cartesian grid predictions were more accurate than spherical grid predictions. This initially surprising result appears to be due to the fact that the wave action transport equation (the governing equation of WAM) is divergence-free in Cartesian coordinates, but this is not the case in spherical coordinates. Furthermore, the divergence error was found to be enhanced in shallow water (where the small nest was deployed) when finite-depth effects such as bottom friction, shoaling, and refraction become important.

This work was carried out at the request of Dr. Bob Jensen of ERDC CHL with collaboration from Dr. Erick Rogers of NRL Stennis. The results of this work were passed on to DoD CWO scientists at the "Introduction to the SWAN Wave Model" workshop.

5.3.3 Emulating Co-Array Fortran with Pthreads

In this core project, Richard Hanson of the Rice SPPT PET team and Stephen Wornom evaluated performance improvements offered by a Fortran 90 API to POSIX Threads (Pthreads). The Fortran interface was previously developed by the ERDC PET program. The test case used was a Jacobi method iterative solution of a Helmholtz equation. The project essentially involved the emulation of a Co-Array Fortran solution using Pthreads. Results were obtained for the SGI Origin 2000, SGI Origin 3000, SUN E10000, COMPAQ ES-40, and IBM Power3 HPC platforms. The timing results showed that the use of Pthreads is a promising approach.

This work was requested by Dr. Alan Wallcraft of NRL Stennis. Dr. Wallcraft also suggested the use of the selected test case.

5.3.4 Enhancement, Evaluation, and Application of a Coupled Wave-Current-Sediment Model for Nearshore and Tributary Plume Predictions

This focused effort (David Welsh, Keith Bedford, Ponnuswamy Sadayappan, and Rong Wang) entailed the continued development of the COupled MArine Prediction System (COMAPS). COMAPS is comprised of coupled parallel-processing versions of the WAM wave model, the CH3D-SED circulation and sediment transport model, and the WCBL wave-current-sediment bottom boundary layer model. In addition to WCBL, COMAPS includes wave-current coupling mechanisms at the water surface boundary layer. The overall aim of the COMAPS project is to improve the accuracy of wave, current, water elevation, sediment transport, and sediment suspension predictions by accounting for previously neglected physical coupling mechanisms. This will lead to better support of military operations such as fleet navigation, amphibious landings, and navigation channel maintenance. WAM and CH3D-SED are production DoD codes in terms of both operational and research activities, so the potential pay-off of this work is highly significant. WAM users at ERDC include Drs. Bob Jensen and Lihwa Lin. CH3D-SED users include Drs. Billy Johnson and Jeff Holland of ERDC.

In PET Year 5, COMAPS bottom boundary layer coupling was upgraded in terms of both convergence reliability and physics. Previous shallow water convergence problems were traced to two factors: A step-discontinuity at the onset of mobile bed roughness contributions, plus excessive sediment-induced stratification. The first factor was addressed by gradually introducing mobile bed roughness and augmenting the standard Newton-Raphson scheme with a Bisection scheme. The second factor was addressed by applying a reduction factor where necessary. This simple approach was found to be more effective than sophisticated solutions. Previous deep water convergence problems were removed by adding a pure current boundary layer branch to WCBL. This branch is followed when near-bottom wave-induced motion falls to an insignificant level. Bottom boundary layer physics was upgraded by modifying the standard SED parameterizations of reference concentration and critical bottom stress to be consistent with the more accurate algorithms used in WCBL.

The COMAPS system will be deployed in the summer 2001 in support of a work unit of the ERDC Dredging Operations and Environmental Research (DOER) program. The particular work unit involves the offshore placement and tracking of dredged material at the ERDC FRF, Duck, NC. The aim of the work unit is to improve the planning and management of Army Corps dredging operations. COMAPS deployment in support of DOER was requested by Dr. Joe Gailani of ERDC CHL. Discussions on this matter have also involved CHL scientists Drs. Jim Clausner, Norm Sheffner, Bob Jensen, and

Rebecca Brooks. Dr. Peter Orlin of the NAVO Ocean Products Division is also interested in using COMAPS in connection with his group's sediment plume projects.

5.4 EQM: Environmental Quality Modeling CTA

(TICAM – Texas)

The activities of the EQM team can be classified into four major categories:

- Coupling of multi-physics codes, treating both theoretical and implementation aspects;
- Identification and presentation of new, novel algorithms for advection/diffusion/reaction with application to environmental modelling;
- Parallelization, debugging, validation, and evaluation of hydrodynamics and water quality codes;
- Enhancements of major environmental modeling software.

5.4.1 Interpolation and Projection Between Arbitrary Space/Time Grids

The UTPROJ3D code has been delivered to ERDC MSRC. The code can handle linear interpolation from TABS-MDS grids to CE-QUAL-ICM grids, mass-correct the corresponding velocity fields, and post-process the solutions for visual interpretation. The code may be run in either serial or parallel environments. UTPROJ3D has been tested on representative velocity fields delivered by the engineers in the Coastal and Hydraulics Laboratory at ERDC. Further testing will be done to evaluate the performance of the code and to determine whether or not the mass-corrected velocity fields meet the requirements of the transport code CE-QUAL-ICM. Two tests have been proposed for the latter: a uniform salinity test and a transport test.

For the uniform salinity (or tracer) test, the plan is to set uniform salinity conditions at all locations with all boundaries set to the same concentration. This test will indicate that volume is being conserved and that CE-QUAL-ICM is properly mapped to TABS-MDS and that hydrodynamic information is being transferred in the correct order.

The second test is a transport test in which the tracer is applied at the same location in both models. A block of grid cells would be given some initial concentration, and the models would be run so as to cause the material to move. The size of the block would increase for each test. The purpose of this test would be to study the manner in which boundary information is handled in each model and to study transport with corrected velocities.

In order to complete each of these tests, velocity information from the appropriate models for a sufficient time period is needed. At present, there is not enough data. These tests will also help to evaluate the performance of the solver routines, as well as better determine the effectiveness of various preconditioners.

5.4.2 Improved Parallel Performance for Environmental Quality Models

CE-QUAL-ICM is a water quality model that has been widely used by EQM researchers at ERDC MSRC and other MSRC and distributed centers. CE-QUAL-ICM is used for evaluation of proposed dredge material disposal sites, such as New York Harbor, and is also used for evaluation of possible releases and transport of contaminants in the upper Chesapeake Bay area. The EQM PET team successfully parallelized CE-QUAL-ICM using software such as VAMPIR (Pallas) for evaluating message passing and I/O efficiencies and PAPI, developed by the Tennessee SPPT PET team, for evaluating MFLOPs on the Cray T3E. The EQM team also worked in conjunction with the Tennessee PET team in using MPI Parallel I/O and MPI Connect I/O for reducing the number of open files in large processor jobs.

Design and implementation of the prototype version of CE-QUAL-ICM, which uses MPI-2 style parallel I/O, has been completed for the Cray T3E platform at ERDC MSRC. Because of the complexity of this project, only one of the important output files has been concentrated on – the so-called averaged plot file (APL). Benchmark comparison of the relative performance of the original code with the parallel I/O is in progress. This work has been a joint PET project with David Cronk at Tennessee.

During the next phase of development, the team will apply the same techniques to as many output files as possible, and to the largest input file, the hydrodynamics data file (HYD), which is typically 1 GB/year of data.

One technical problem not foreseen is that the MPI-2 output file is not a native binary (COS file on T3E), and this needs to be dealt with to make it compatible with existing post-processor software used by ERDC MSRC. Solutions to this problem are being discussed.

5.4.3 Transport Schemes for Water Quality Modeling

A recent focused effort has been to investigate and develop conservative, higher-order accurate methods for advection and diffusion, suitable for any type of elements. The methodology to be investigated was based on the so-called discontinuous Galerkin methods (DGM), which have been developed by Wheeler, Dawson, and their collaborators.

This new scheme has been implemented into the parallel CE-QUAL-ICM code. The scheme uses second-order Runge-Kutta time integration and piecewise linear discontinuous finite elements with slope limiting in space. The combination of second-order approximation with slope limiting should provide higher accuracy while maintaining stability of solutions. The new scheme has been integrated into the existing code data structure and requires the change of only one control parameter to be run. The EQM team also provided EQM users at ERDC MSRC a prototype three-dimensional advection-diffusion code on unstructured grids based on the DGM methodology.

5.4.4 A Full 2-D Parallel Implementation of CH3D-Z

CH3D-Z is a three-dimensional hydrodynamic model widely used to investigate important hydrodynamic processes in rivers and coastal areas. In particular, it has been used for studying the impact of contaminant releases, navigability of naval shipping lanes, and channel deepening. It has also been coupled with a water quality model to study water pollution problems, for example, in the Chesapeake-Delaware Bay region.

Several attempts have been made to parallelize and thus improve the performance of CH3D-Z. The original version of the code used an operator splitting approach for computing depth-averaged velocities and elevation. In this approach, an x-sweep was performed to compute the x-velocity and intermediate elevation, followed by a y-sweep to compute the y-velocity and elevation at the next time step. This sequential approach does not lend itself to parallelism, and thus most previous attempts to parallelize the code used a one-dimensional domain decomposition, which in general will not scale well.

A full two-dimensional domain decomposition parallel implementation of CH3D-Z has been attempted. The first part of this project involved replacing the operator splitting algorithm described above with a more fully implicit approach, whereby elevations are computed using a full two-dimensional linear solve. This linear solve involves a symmetric, positive definite matrix, thus a preconditioned conjugate gradient algorithm was employed. This work was completed in summer of 2000, and the new code was tested and compared to the previous version of CH3D-Z for both the Chesapeake Bay-Delaware Bay data set as well as the lower Mississippi River data.

The parallelization of the new version of the code has proceeded in the following steps:

(1) A pre-processor was written to split the computational domain into subdomains (using METIS), and to split the physical data into subdomain data to be read by each processor;

(2) MPI calls have been added to the code for message-passing purposes.

The primary efforts have been to parallelize and verify the correctness of the code from start-up through one step of the two-dimensional linear solve, as this appears to be the primary bottleneck preventing parallelization. It has been verified that for a two-subdomain decomposition, the parallel code obtains the same elevations and depth-averaged velocities as the original serial code through one time step. The next step is to complete the parallelization of the remaining subroutines and verify the correctness of the code over several time steps. This process is expected to be complete by the end of summer 2001.

One of the major difficulties in parallelizing CH3D-Z is the amount of hard-wiring that has gone into the code to handle certain special cases. For future portability of the parallel code, some attempt will need to be made to create a clean, generic version of the code upon which future versions can be based.

5.4.5 Dual-Level Parallelization of MGPOM

The Princeton Ocean Model (POM) is widely used by the U.S. Navy for coastal ocean circulation simulation. The EQM team successfully converted the single-block-grid POM code into the multiblock grid code (MGPOM). MGPOM was parallelized using MPI, since not all grid blocks are of the same size, and OpenMP/Pthreads was used as a second-level parallelism for improving load imbalance produced by MPI processes. The MPI-OpenMP version of the MGPOM code was used for the simulation of the Arabian Gulf. Performance results from this version show a speedup of 57X on the 20-block rectangular grid and 61X speedup on the 42-block curvilinear grid with nearly double the horizontal grid resolution. Performance results of the MPI-Pthreads version for the U.S. West Coast simulation on the 29-block rectangular grid show a speedup of 41X.

5.4.6 FEMWATER Visualization and Data Management of Very Large DatsSets

Parallel FEMWATER Visualization, a PET focused effort project, was funded to develop readers for FEMWATER files for the Ensight visualization software package. This included the development of FEMWATER files for two military material storage sites for Dave Richards in the Groundwater Modeling Technical Support Center at ERDC, the creation of FEMWATER to Ensight reader files, the creation of an Ensight FEMWATER tutorial, and the development of film loops. These efforts resulted in a new series of useful visualization tools for the GMS user. The team sent Drs. Stacy Howington and Jeff Holland these tools as they were developed. The files created during the summer were imported into Ensight to test these tools. Stacy Howington reviewed the multi-platform tools and agreed that they should be placed on the Web site for all GMS users.

Parallel FEMWATER Data Management, a PET focused effort project, was funded to develop readers for FEMWATER files for the HDF5 data management software package. The team was able to successfully convert FEMWATER files to HDF5 files. Sub-setting was also explored for visualization using Ensight. Sub-setting can be performed in combination from FEMWATER to HDF5, with linkages provided by the teams but still cumbersome. The team received programs from NCSA for conversion from HDF5 to Ensight. (This conversion program was developed with the aid of Mike Folk of the NCSA SV PET team and Kent Eschenberg of ERDC MSRC.) These have been tested and found able to convert HDF5 files into Ensight files. In addition, the team has developed a preliminary tutorial. Although the programs have been successfully linked, the process is still awkward. The team is very near to providing a translation reader from HDF5 into FEMWATER files after sub-setting. Preliminary testing using a Web server (ArcIMS) to serve data on-line has been tested, but needs further analysis.

The team is developing a simplified unified program that will make the FEMWATER/HDF5/Ensight translation process easier for the user. A new tutorial will be developed for this unified program and posted on the Web site for all users. It will also be posted on the ListServ developed for user interaction.

5.5 FMS: Forces Modeling and Simulation/C4I CTA

(Syracuse)

One focused effort project was funded in Year 5 in the FMS area by ERDC MSRC PET (whereas ARL MSRC PET provided FMS core support). The ERDC MSRC project was focused on SPEEDES Installation and Training at ERDC MSRC. Syracuse had previous experience with SPEEDES (Synchronous Parallel Environment for Emulation and Discrete-Event Simulation) while the system was under development in an FMS CHSSI effort at Metron Corporation in San Diego. Assistance was provided to SPEEDES-based CHSSI FMS projects, and installations of early versions of SPEEDES (v0.6 - 0.9) on Origin2000 systems at ERDC MSRC, ARL MSRC, and NRL. Last year, SPEEDES was adopted by JSIMS as the core simulation engine. As part of this focused project, monitoring the complex transition process of SPEEDES to JSIMS was initiated by Jeff Wallace (at this time at SPAWAR San Diego and Technical Director of JSIMS Maritime) and David Pratt (at this time JSIMS Technical Director). SPEEDES is a government – owned (NASA) software system, with Metron having a special development license. However, JSIMS selected another San Diego company, RAM Labs, to continue support for the JSIMS version of the system. Consequently, there are currently two competing versions of SPEEDES: the Metron version, sponsored by the Wargame2000 Project at the Joint National Testing Facility at Colorado Springs, Colo. and the RAM Labs version, sponsored by JSIMS enterprise and CHSSI FMS-5.

As part of the Year 5 focused effort project, the ERDC MSRC PET team established contact with both companies; received both versions of the system; analyzed the available documentation; performed source level analysis of similarities/differences between the two versions; consulted major players in the SPEEDES domain; and developed a strategy for the Year 5 SPEEDES training development and delivery. Since the current (early) JSIMS version offers support only for Solaris and Linux, and the more mature Metron version offers a genuine multi-platform support (including IRIX), the Metron version was selected as the tentative target for the Year 5 training. A suite of about 10 tutorial applications, distributed as part of the Metron release, was analyzed and adapted for the ERDC MSRC training needs. However, because new emergent features such as Federations Objects were covered by the JSIMS version, some of the JSIMS tutorial examples were converted to the Metron version. The SPEEDES Tutorial was delivered to ERDC MSRC in March 2001, and the Metron version of the system was installed on the Origin3000 at ERDC MSRC. A port of the JSIMS version of SPEEDES to the SGI Origin platform is in the works.

5.6 C/C: Collaboration and Communication

(Florida State)

5.6.1 Communication and Collaboration Core Support

One highlight of the C/C core support was the organization of a workshop on the integration of Grids (large distributed systems) with hand-held clients and mobile resources (sensors). This was originally planned for the summer of 2000, but the task proved difficult due to the large gulf between the wireless and grid communities – a problem the workshop will address. The meeting will be held May 20-22, 2001, at NCSA. Technology speakers will include Dan Reed (NCSA), Larry Smarr (UCSD), Brad Myers (CMU), Al Gilman (Wisconsin), and scientists from Motorola. Also covered will be the FCC view and applications including distributed wireless sensors for environmental science, wiring remote regions, and hand-held devices for control of visualization devices.

ERDC MSRC PET has supported much of the work in collaborative systems over the last five years, and during that time there has been remarkable progress in base Internet (Object Web) technology, new standards, and commercial environments. This was documented in a survey of commercial and academic tools and the underlying technologies for collaboration. There are now several commercial systems such as Centra, WebEx, Placeware, and Latitude that support capabilities similar to the Tango system, which was first used for remote teaching at Jackson State through PET in the fall of 1997. They have remarkable similarities in architecture and user interface, and this consensus suggests it is low-risk to adopt either one of these or other tools with a similar shared object paradigm.

An audio/video conferencing subsystem was developed using Tango, but this has evolved into a separate area in which it is best to adopt one of the many good stand-alone systems. These can be classified into three broad areas: high-end or community, specialized point-to-point, and desktop. The Access Grid developed at Argonne was recommended with NCSA support, for a high-end system. This features multiple video streams and large screen display, and requires good quality 20 megabits/sec network links. One interesting low-end audio standard is HearMe which supports the integration of multi-point telephony and Internet. An operational server is at FSU, and Access Grid systems are being installed at FSU (2), ERDC MSRC, and Jackson State. A later focused effort describes this in more detail.

XML is growing in importance with better tools and new object standards. Initially, XML was aimed at separating the specification and rendering of information; in particular it allows a document to have a single XML specification of its information content but be rendered in different ways, such as with a hand-held device or workstation. XML is now being used as a universal object specification with the new "Schema." There are several important XML applications for database, and general scientific data that could, for instance, help interoperation of codes and tools, which is particularly important in multidisciplinary problems. As an example of XML standards, SVG Scalable Vector Graphics for 2-D scientific visualization was cited, RDF for Metadata, SMIL for multimedia training data, and MathML for Mathematics.

5.6.2 Training Core Support

An in-depth review of major synchronous and asynchronous collaboration tools was conducted with a special study of the additional capabilities needed for education and training. Collaboration supplies shared documents and audio/video conferencing. The paradigm for this is now well established, and either server (Web) or local applications can be shared. The latter is best done using the shared display technology typified by NetMeeting from Microsoft, with better implementation from other vendors (Centra, Placeware, WebEx). Applications range from the shared Web page (first done well by the Tango system supported by ERDC MSRC PET) to the more general shared export model in which custom shared browsers for chosen export formats can be built. The shared printer (equivalent to shared PDF) is an attractive feature of WebEx. This capability can be expected to improve as these new ideas are developed, but even now the commercial support for shared documents is excellent. With the three-tier approach to audio/video conferencing under the C/C core and later focused effort, several reasonable choices exist, although there are weaknesses in support of recording and of interoperability through H323 and SIP standards.

Two key issues for training are authoring and management/administrative systems. The latter includes user registration, homework submission and grading, as well as management of curriculum modules. Both WebCT and Blackboard support these features with some links to university databases, but this feature does not seem as important to training. This perhaps explains these two product’s popularity with universities but not in corporate training. It is not expected that these systems will remain competitive due to their weak authoring model. Rather, there will be a growing trend to use high-end authoring systems such as those from Macromedia and Adobe. Here, systems such as Flash and Illustrator are built around careful layout for which SVG provides a common standard supporting interchange among the competing high-end systems. Support of standards should lower the risk – in wasting effort developing course material in dead-end proprietary formats – for investing in high-quality curricula pages.

An important development is the maturing of the IMS (academia) and ADL (DoD) standards, which specify the structure of training modules and the user administrative data associated with education and training. These standards have not been proven and have some obvious limitations: they are built around an old-fashioned client/server model for computing: rather than the multi-tier architecture used in modern Object Web systems including those built at FSU and Syracuse. Nevertheless, these standards are very valuable in making clear what metadata needs to be specified and what the basic training object characteristics are. Similar efforts are appropriate to specify HPCC and Science object standards.

5.6.3. Ubiquitous Access to HPC Resources

Louis Turcotte, former government PET Lead at ERDC MSRC, produced a survey (in the form of a PowerPoint presentation) exploring the different uses for small devices. The main reason for this is the expected confluence of the cell phone and the personal digital assistant as universal wireless portable systems. It has been estimated that by 2005, 60 million Internet-ready cell phones will be sold each year and that 65 percent of all broadband Internet accesses will be via non-desktop appliances. This suggests that hand-held wireless devices will play a important role in areas now dominated by desktop clients, enabling new applications and new approaches to old applications. In this focused effort, palmtops could be used to support high performance computing and training applications. Also studied were some of the base technologies building on earlier work in PET using WAP and WML protocols. The "Grid on the Go" conference is also expected to be important in refining the general understanding of how wireless devices will interact with computational and education grids. The new Bluetooth is seen as a standard to enabling pervasive short distance wireless links. This and the new protocols should enable construction of hand-held optimized Web sites by a broader community, with a need to move away from the current "closed garden" approach typified by Palmnet where the wireless Web sites are high-quality but proprietary.

A simple architecture was designed in which palmtops interact with an adaptor or personal server that mediates between the desktop and palmtop capabilities. For instance, where a shared display may be downsized from a desktop to match the smaller palmtop screen. The latest release of VNC (public domain shared display) for palmtops is quite impressive – it is fast and includes server side resizing for reducing the shared display size. Analogously, the intermediate adaptor can simplify shared export XML files such as HTML or SVG so they can be handled by the less powerful palmtop. This way, palmtops can be included in collaborative sessions such as those involved in training. Students can get quizzes, Web page summaries, and assignments on their palmtops while watching the full curricula on a large, high-quality display. As another example, FSU and the visualization group designed a demonstration of wireless palmtops that control high-resolution displays, producing a much more powerful personal interface than the conventional untethered mouse and keyboard interface. Interfacing palmtops using an adaptor to a portal like Gateway from FSU can support job submission and status monitoring from HPC systems. The Garnet portal supports shared display, instant messenger (from the open source Jabber.org), text chat, and shared SVG and HTML files.

5.6.4 Collaborative Portals for Training and Computational Science

This project is developing technology and associated demonstrations of advanced collaboration systems that build on experience using the Tango Interactive environment as well as the current generation of commercial systems Centra, Placeware, and WebEx. Portals allow users to manage and display objects in a 3-tier model, while collaborative systems allow shared objects. It is natural to combine these concepts in a collaborative portal using a common object specification. This allows the user to find objects, render them and know what properties to share in what fashion. A prototype of the Garnet collaboration system, with a novel architecture and several new capabilities, has been designed and implemented.

Key Garnet capabilities include support of collaborative sessions involving any mix of devices including desktops, CAVE's (high end visualization devices), and hand-held clients. Garnet also allows integration of asynchronous and synchronous collaboration with a universal archive service supporting later replay. A common XML specification invoices both managing and sharing objects. During replay of audio/video in streaming codecs (such as RealNetworks), the standard low latency conferencing codecs (such as G.711 for audio) can be recorded. Rather than the shared browser of Tango, the shared display (framebuffer) is the default method of sharing documents. This is augmented by a shared export capability supporting specialized displays of important formats. Natural choices include HTML (basic shared browser), SVG (2D vector graphics), and PDF (or printer). More specialized shared export possibilities are Java2D/3D and Java Server Pages (JSP). This allows support in both education and computing collaborative portals. The XML object specification will be consistent with the IMS and ADL education and training standards. Shared display and shared JSP allow support in collaboration for both job submission and visualization for the Gateway computing portal.

Looking at the underlying technology, an important idea is the use of a common publish/subscribe message service for both asynchronous and synchronous messaging. This has not been used in major systems before but is very helpful in the integration of asynchronous and synchronous collaboration. Of existing commercial messaging systems, the JMS (Java Message Service) system SonicMQ from Progress Software has been found to be the best available with lowest latency (about a millisecond for small messages) and the best bandwidth of four products evaluated. A designed optimized message service for this type of application has been proposed as a candidate Grid Message Service. This includes full support for XML messages and the use of server side software filters in selecting messages. This work, supported by ERDC MSRC, will be the topic of the June 2001 Syracuse Ph.D. thesis of Pallickara. In this approach, archiving (persistent messages) is achieved with a database that subscribes to all messages. A further universal event specification, is designed to support general collaborative portals with compatibility with IMS, ADL and other application specific standards.

Tango ambitiously built a fully integrated system, which is no longer practical as with an aim at greater functionality and to build systems of greater technical complexity. A modular structure is used to take components from best practice and focus on key innovations for our contribution. The team will build on existing implementations for the audio/video conferencing, message service, and base shared display infrastructure. In the case of the message service, new approaches (as in Grid Message Service discussed above) are being researched and will substitute our technology when it is more mature.

Garnet has been designed to use either Argonne's Access Grid or the commercial desktop HearMe system. This implies that FSU would replace the shared PowerPoint capability of the Access Grid with the more powerful shared object model from Garnet. Other audio/video systems will be linked to Garnet as required and as experience builds.

Garnet, like Gateway, uses XML extensively for all interfaces and message specification. The middle tier is built using Enterprise Javabeans rather than Corba as used in Gateway.

5.6.5 Modular Collaborative Environment

This focused effort studied the Access Grid and HearMe audio/video systems in detail. The Access Grid (AG) was originally developed by Argonne but has been extended as part of the NCSA Alliance. There are now more than 50 of these high-end audio/video conferencing systems installed worldwide. Two systems are being installed at FSU under ERDC MSRC PET – one fixed and one transportable model aimed for "teachers" in a distance education scenario or for use in a small conference room. The Access Grid is described at http://www.mcs.anl.gov/fl/accessgrid/ and training sessions are available. NCSA recently offered AG training to ERDC MSRC personnel at the Access Center in Washington, and it is expected this can be arranged for all the major PET and MSRC sites that wish to install AG nodes. A "train the trainers" model is intended, so that once a cadre of experts exists at HPCMO/PET sites they can help other sites in this community. This will build a critical mass of AG systems to enable electronic collaboration to be effective in HPCMO/PET. Currently ERDC, JSU, and ARL intend to have AG installations.

Although the AG is an impressive system, there are some issues to address. It is recommended that different shared document systems be used when the simple shared PowerPoint of the AG is insufficient. The AG community should look at H323 or SIP (the audio video interoperability standards) compliance for this technology. This would allow the user to support hybrid sessions involving simultaneous systems such as AG, PictureTel, Polycomm, CUSeeMe, and HearMe. Finally, clients support should be partitioned so that multiple communities can be separately administered. Also an important (for HPCMO) recent enhancement to the AG supports encrypted media streams.

HearMe http://www.hearme.com is a low-end audio conferencing system supporting a general mix of phones and Internet clients with participant control. The phone option is helpful as it allows audio communication with better quality of service than can be guaranteed on the Internet. The phone and Internet options are integrated, as both are converted to the same codecs and recorded for later replay through the Web. FSU is adding SMIL-based replay of session (the W3C standard for multi-stream, multi-media files) by converting G.711 or G.723 codecs digitized on the HearMe server to RealAudio. A HearMe server installed at FSU has a license for 20 simultaneous users.

The Access Grid produces a "designed space" aimed at supporting groups interacting with groups – PictureTel or desktop systems are more optimized for individual interactions. The AG features hands-free high-quality audio, multiple video and audio streams, and life-size displays. Four PCs control it, and AG equipment includes an echo canceling box, multiple camera, and projector or frame buffer displays (at least three). HearMe provides two types of conferences: standard and moderated. In the standard conference, every client has the same privileges and can speak at any time. In a moderated conference, there are three types of users: moderator, panelist, and participant. The moderator is the creator of the conference and has full control over the session. Panelists are those given the right to speak while participants can listen but need the permission of the moderator to speak.

5.6.6 Computational Science and Information Technology: Curriculum and Education

This focused effort brought together the issues needed for training and education over and above the collaboration (shared document and audio/video conferencing) systems covered in other projects. PET originally planned to offer a course in Spring 2001, but this was postponed. The issues include curriculum, delivery, and authoring.

The delivery can be implemented using the Access Grid (preferable if possible) or desktop conferencing such as HearMe. The FSU, ERDC, and Jackson State AG deployment could be tested by delivery of distance classes or training sessions. Garnet is designed to support both the advanced authoring (Macromedia Flash) and management standards (IMS, ADL) described below.

Over the past year courses have been offered both in simulation (parallel computing) and information (Internet) technologies. These are both needed as many fields are now integrating both issues. For instance, a user needs XML-based technologies to record data and assimilate this into large-scale simulations. As seen in portals, a user needs modern management technology to keep track of the increasingly complex process of computation. There are three major online core courses from the past year and a half: CPS1: http://old-npac.csit.fsu.edu/projects/cps615spring00/ (computational science taught at ERDC Graduate Institute, Spring 2000) and two new courses from FSU: IT1 at http://aspen.csit.fsu.edu/it1spring01/ and IT2 at http://aspen.csit.fsu.edu/it2spring01/. IT1 IT2 update information technology courses that were very popular when taught from Syracuse to Jackson State from 1997-2000 in ERDC MSRC PET. They are supported by an online technology resource http://aspen.csit.fsu.edu/windsnow/webtech/. The last course, IT2, has particular focus on XML, which is very useful in defining the interoperable datastreams and interfaces needed for multidisciplinary applications.

The curriculum used in distance education needs “only” to be Web-based. Currently, most of our team’s experience has been with simple authoring tools such as basic HTML, exported PowerPoint, WebCT and Blackboard. The latter two commercial systems produce visually appealing pages that typically lack rich multimedia and interactive characteristics. The team is encouraged by the developments of standards such as SVG (XML-based standard format for 2-D vector graphics). The best authoring products from Adobe and Macromedia should soon support this format (there is a prototype Flash to SVG convertor, and Adobe Illustrator allows SVG output). Such a development would allow the user to develop high quality Web pages and export using standards compliance to guarantee that the content will survive changes in vendors and products moving on Internet time. It is suggested that users look at core courses (MPI training, base Java course above) and spend the effort to author them in a more interactive format. Courses whose content is still changing rapidly should probably stick with approaches such as PowerPoint, which require less investment in authoring.

ADL (http://www.adl-net.org) and IMS (http://www.imsproject.org) have produced learning object standards that address the structure of curricula above the Web page. They define a natural hierarchical arrangement, discussing the metadata that link pages to course modules and define prerequisites, objectives, and completion requirements. There are also standards for user-related data (administrative and grading), as well as tests and quizzes. ADL and IMS standards currently have no overlap with the authoring issues discussed above, making it sensible to pursue both goals – high quality authoring and standards compliant learning objects – simultaneously.

A common type of page includes basic “content” surrounded by “decoration.” The decoration would be advertisements or pointers to other Yahoo goodies for a Yahoo portal page. For an education page, (such as those produced by WebCT, Blackboard, FSU), the decoration is a group of buttons accessing services such as “chat room,” “class resources,” “send mail to instructor,” WebTop Services (search etc.) and links to other content (Next, Previous, More Detail). This page structure is best thought of as a portal. The curriculum part is classified as a unit in IMS or ADL. The decorated page should not be directly stored but generated when the portal is invoked.

In summary, FSU has developed a strategy that supports the emerging object standards, high quality authoring, portals, and the best delivery systems. This is recommended as best practice.

5.7 SPP Tools: Scalable Parallel Programming Tools

(Rice and Tennessee)

5.7.1 Rice

5.7.1.1 Fortran API to Pthreads

The goal of this project was to bring basic thread programming technology to the DoD Fortran applications programmer. During the year, Clay Breshears, Henry Gabb, and Richard Hanson completed work on a software package and a paper that accomplished this goal. The fruits of this work will become available after publication. The review process is still under-way in *ACM-TOMS*. The software package is portable. A small set of changes to the package allows the API to be used in any Unix or Linux programming environment that supports POSIX Threads, or Pthreads. Ports to SGI Origin, IBM Power3, SUN Enterprise, Compaq ES40, and Linux systems are included, with testing software provided.

5.7.1.2 Developing Multi-Threaded Fortran Applications Using the PARSA™ Software Development Environment.

This focused effort by Jeff Marquis and Geoffrey Wossum of the University of Texas at Arlington addressed the potential of multi-threaded Fortran applications using the PARSA™ Software Development Environment. The PARSA programming methodology and its associated tools give DoD HPC users an easy-to-use, fast, and efficient method for developing Fortran projects that exploit the resources of shared memory systems. Developing multi-threaded projects using directives-based programming methods puts additional development requirements on programmers, driving up the cost, time, and expertise needed to develop software projects. The PARSA programming methodology, however, does not put additional development requirements on software projects but produces scalable and efficient multi-threaded software. The PARSA programming methodology allows programmers to exploit many different forms of parallelism using different types of graphical objects supported by PARSA. A Fortran-Pthreads application programming interface (API) is introduced that allows PARSA programmers to embed Fortran-like threading directives into their Fortran projects if needed. An example Fortran project is presented in the ERDC MSRC PET Technical Report from this project that demonstrates how easily multi-threaded Fortran projects can be developed in PARSA.

5.7.2 Tennessee

5.7.2.1 Parallel I/O

As processing speed increases, I/O is becoming a bottleneck for certain classes of applications. This project studied the use of the MPI-I/O extensions as a method of easing the I/O bottleneck through the use of parallel I/O. While time was taken to learn and understand the use of MPI-I/O, particular emphasis was placed on applying this to existing DoD applications.

LBMPI is a Contaminant Dispersion Model EQM Challenge code being used by Robert Maier at the Army HPC Research Center (AHPCRC). The code performs computation using what are conceptually four three-dimensional arrays. In practice, however, the four three-dimensional arrays are stored as a single four-dimensional array. This is done to achieve a better cache-hit ratio. The application uses a block-block data distribution with layers of ghost cells. This code was experiencing a severe I/O bottleneck. Running on an IBM SP2 using 512 processors, a typical run required approximately 12 hours of compute time and an additional 12 hours of I/O time. The traditional Unix-style I/O calls in LBMPI were replaced with parallel I/O calls using the MPI-I/O extensions. This resulted in an I/O speedup of 92 when running on 32 processors.

CE-QUAL-ICM is an EQM code developed at ERDC and being worked on by Victor Parr of the EQM PET team at TICAM. The code performs computation using a large number of arrays, with the parallel version distributing the arrays in an irregular fashion. These arrays also contain a high percentage of ghost cells (typically 20-35 percent).

Typical production level executions perform 10-year simulations. The current solution has each process write results to separate files. This is followed by a post-processing step that must re-read all the output data, re-organize the data, and write the data to a single final output file. A solution that does not require this post-processing step is desired, and a solution using MPI-I/O has been designed and implemented. A solution using MPI-I/O has been designed and implemented. This solution eliminates the post-processing step and should lead to improved performance. Performance results have not yet been collected.

By introducing DoD users to parallel I/O, the I/O bottleneck being encountered by many applications can be greatly reduced. This will result in users being able to run larger and longer simulations, thus improving efficiency.

5.7.2.2 Metacomputing Support for the SARA3D Structural Acoustics Applications

This project uses the NetSolve MATLAB interface to provide remote access to HPC platforms for users of the SARA3D structural acoustics code. NetSolve is a client/server system that provides access to HPC hardware and software from familiar desktop environments using a variety of client interfaces. SARA3D is a finite element program for computing the frequency response of general three-dimensional structural acoustics problems. SARA3D solves the time harmonic problem of a structure submerged in an infinite fluid subjected to incident traveling waves or to vibrational loads within the structure. Separate fluid and structure models are created and connected via coupling elements. The coupled fluid/structure model results in a complex, symmetric, banded set of equations that can be efficiently solved by Gaussian elimination for displacements and pressure throughout the model. Far-field or near-field pressures can be computed from the normal velocities and pressure calculated on the surface of the structure.

NetSolve is being used to provide real-time response for post-processing and visualization of large-scale SARA3D output data. SARA3D has been implemented as a NetSolve service that runs on HPC machines. SARA3D can be invoked remotely from the NetSolve MATLAB or Fortran or C client interfaces on the user's workstation. The SARA3D input file is transferred by NetSolve from the client to the server, and the SARA3D output is transferred from the server to the client when the SARA3D computation is finished. Non-blocking NetSolve calls can currently be used to obtain coarse-grained parallelism. Current work involves developing a mechanism for persistent file storage between runs so that results of previous SARA3D runs can be used as input to subsequent post-processing requests, as well as handling output file partitioning and distribution to support concurrent post-processing by distributed processes. Other current work involves achieving additional parallelism through use of the NetSolve task farming interface. Future work will investigate how to integrate the interactive NetSolve interface with batch queueing environments.

5.8 Scientific Visualization

(NCSA – Illinois)

5.8.1 Standard File Format for Large Data Problems and Visualization

This project studied the applicability of the HDF5 file format and I/O library to address the need to improve storage efficiency and data access speed when dealing with very large data sets generated and used by projects that use the ERDC MSRC. This involved a number of training sessions, consultations with potential users, porting the HDF software to specific platforms of interest, and development of standards for organizing user's data within HDF.

The project began with two training sessions, in which potential users were trained to use HDF5 and were exposed to the capabilities of the technology. From this activity, a number of potential projects were identified and pursued. For example, the NCSA team ported the HDF5 Fortran API to the Windows Visual Fortran environment in order to better meet the needs of the MSRC customers. The team also hosted PET collaborators from Texas A&M University at Kingsville to consult on using HDF5 with FEMWATER. An HDF5 reader for the visualization tool Ensight was delivered to the Kingsville team. Finally, a draft standard for time-varying structured and unstructured data was generated in collaboration with visualization personnel at the ERDC MSRC Scientific Visualization Center.

5.8.2 Visualization for EQM

The objective of this focused effort was to support the ERDC team led by Dr. Carl F. Cerco in its use of the EQM dataset visualization tool, CbayVisGen Version 3.1. CbayVisgen Version 3.1 was developed by NCSA and transferred to ERDC MSRC in prior years of PET. In Year 5, the tools have been enhanced to include visualization of observed data. This allows the user team to look at data gathered from Chesapeake Bay within the spatial and temporal context of the simulation output. Solutions have been addressed about the issue of visualizing very large datasets, especially the output of long-running scenarios. Recent success in the distributed calculation allows ERDC scientists to conduct simulations of more than 10 years. These large runs produce output that is too large to download to the local workstation for visualization. FSU has experimented with the possibility of decomposing the visualization tool into client and server components. Heavy lifting would be done on a high-performance server machine, with results sent to a lightweight client running on the user's local workstation.

6. Tools Introduced into ERDC MSRC

The enhancement of the programming environment at ERDC MSRC through the identification and introduction of programming tools, computational tools, visualization tools, and collaboration/communication tools is a major emphasis of the ERDC MSRC PET effort. Tools introduced into ERDC MSRC by the PET team during Year 5 are described in this section. Other tools installed in previous years are described in earlier reports and are continually supported. The ERDC MSRC PET team has provided training courses at the ERDC MSRC and at remote user sites for many of these tools (see Section 8), and continually provides guidance and assistance in their use through the on-site team. Many of these tools came from collaborative efforts across various components of the ERDC MSRC PET team, both on-site and at the universities.

6.1 Programming Tools

6.1.1 FPTHRD - Fortran Pthreads API Package

The primary programming tool suite completed during Year 5 was the Fortran Pthreads API package, FPTHRD. This package now covers the platforms SGI Origin, IBM Power2, SUN Enterprise, Compaq ES series, and Linux clusters, with a single compiler choice. Any application code written for one of these platforms, with respect to FPTHRD, will run on any other. An exception is the Linux cluster where the implication is in one direction: Running on Linux implies running on the alternates, but not conversely.

Prospects are good that FPTHRD will be available to the widest possible audience, provided it is accepted as an Algorithm by *ACM-TOMS*. This will be through *netlib*, which automatically follows publication. Review of the paper and code package is ongoing.

6.1.2 PAPI

PAPI is a specification and reference implementation of a cross-platform application programmer interface to hardware performance counters. These counters exist as a small set of registers that count events, which are occurrences of specific signals related to a processor's function. Monitoring these events has a variety of uses in application performance analysis and tuning. The PAPI specification consists of both a standard set of events deemed most relevant for application performance tuning, as well as both high-level and low-level sets of routines for accessing the counters. The high-level interface simply provides the ability to start, stop, and read sets of events, and is intended for the acquisition of simple yet accurate measurement by application engineers. The fully programmable low-level interface provides sophisticated options for controlling the counters, such as setting thresholds for interrupt on overflow, as well as access to all native counting modes and events. It is intended for third-party tool writers or users with more sophisticated needs. PAPI has been implemented for all ERDC MSRC platforms and is installed on the Cray T3E and the Origin 3000. Installation of an AIX kernel extension on the IBM Power3 SMP is required before PAPI can be installed. PAPI is currently being used to tune EQM codes on ERDC MSRC machines. Incorporation of support for PAPI into the Vampir MPI performance analysis tool and the GuideView OpenMP performance analysis tool, as well as into a new combined MPI/OpenMP performance analysis tool called VGV (Vampir-GuideView) is currently under way. Use of PAPI by these tools will allow the general ERDC MSRC user community to take advantage of the performance metrics provided by PAPI.

6.1.3 MPI-2 I/O

MPI-I/O provides a library interface for performing parallel I/O. This tool is part of MPI, and as such, is delivered by the MPI vendors for each machine. The use of MPI-I/O provides dramatic improvement in performance for certain classes of applications. As part of the Parallel I/O focused effort, Tennessee tested the vendor implementations of MPI I/O on MSRC machines and taught a training course on using MPI-I/O.

6.1.4 NetSolve

NetSolve is a client-server system for accessing hardware and software resources over a network. NetSolve, developed at the University of Tennessee, enables access to HPC resources from familiar desktop environments, using a variety of client interfaces, including Fortran, C, and Java programming interfaces and MATLAB and Mathematica interactive interfaces. Non-blocking NetSolve calls enable coarse-grained parallelism without requiring users to write any actual parallel code. The NetSolve task farming interface provides another convenient way of obtaining parallelism. A Year 5 focused effort has demonstrated the usefulness of NetSolve for providing access to HPC resources for users of the SARA3D structural acoustics code. If NetSolve can be integrated with the queueing systems on MSRC machines, it has the potential of enabling transparent access to these resources from the desktop for DoD users of MATLAB and other popular desktop problem-solving environments.

6.1.5 SRCUTILS

SRCUTILS is a small collection of codes used to convert Fortran 77 to Fortran 90 and assist in code maintenance. These codes include *ftof90,* which reformats Fortran 77 fix format code into Fortran 90 free format code, *printps,* which generates Postscript listings of codes, and *dos2unx,* which converts MS-DOS format code into Unix formats. These codes are designed to automate some of the tasks involved in code conversion and are designed to support large programs that might contain hundreds of separate subroutines and functions.

6.1.6 cproto

cproto is a public domain utility for extracting "prototypes" from C code. Prototypes represent the type declaration of a function and its arguments, allowing for type-safe checking. This utility is used in the Beggar code *makefile* system to automate the process.

6.2 Visualization Tools

6.2.1 Windows Visual Fortran Version of HDF5 Fortran API

This tool is a port of the HDF5 Fortran interface to the Windows Visual Fortran programming environment. The port was requested by the Texas A&M-Kingsville PET team, in support of its work with the ERDC Coastal and Hydraulics Lab.

6.2.2 CBay Visualization Tool, Version 3.1

This new release of the CBay Visualization tool includes the ability to visualize observed data. This capability was requested by the user team led by Dr. Carl Cerco of ERDC.

6.2.3 Ensight Reader

The Ensight reader includes seven FORTAN programs that convert FEMWATER files to Ensight format. These include *gm2.for* (geometry); *gm3.4* (pressure head-steady state); *gm5.for* (velocity-steady state); *gm6.for* (concentration-steady state); *gm7.for* (pressure head-dynamic); *gm8.for* (velocity-time dependant); and *gm9.for* (concentration-time dependant). After the files are converted to Ensight format they can be imported into the software and manipulated in the visualization tools. The addition of this capability for the MSRC is significant since it will provide the supercomputer user access to visualization software on the supercomputer platform. These tools are currently being used by Stacy Howington at ERDC to visualize FEMWATER models of military sites. FEMWATER visualization in Ensight software is now available for all users of PCs (Windows NT), workstations, and supercomputing.

6.2.4 HDF5 Reader

The readers include programs to translate FEMWATER files into HDF5 for sub-setting and readers from HDF5 to Ensight for visualization. Readers are also being developed for the translation of HDF5 to FEMWATER. These readers are written in C, the language of HDF5, and one of the most flexible and widely known languages for database manipulation. The purpose of the tools is such that users of FEMWATER on multiple platforms, either supercomputer or workstation, can:

1. Sub-set FEMWATER files for detailed analysis, calibration, or reduction in run time;

2. Visualize the spatial and non-spatial results of the data sub-sets.

This will greatly help the users of FEMWATER for sub-setting and visualization. Until these linkages were made, HDF5 was recognized as an excellent means to sub-set very large data sets, but FEMWATER could not be placed into sub-sets. In addition, the analysis of FEMWATER runs could not be visualized. The readers developed by the team link for the first time the power of sub-setting of HDF5 and visualization using Ensight.

6.3 Collaboration/Communication Tools

6.3.1 Access Grid

This high-end video conferencing system is being installed at both ERDC MSRC and JSU, and is already in place at several PET team sites (NCSA, OSC, FSU).

6.3.2 HearMe

This low-end desktop audio conferencing system is installed at FSU, and its use was demonstrated at a March 1, 2001, PET tutorial at ERDC MSRC.

6.3.3 Centra, Placeware, WebEx

FSU helped ERDC MSRC evaluate Web-based collaboration systems and demonstrated all three of these at a March 1, 2001, PET tutorial at ERDC MSRC.

6.4 Computational Tools

6.4.1 Genie++

Genie++ is a grid generation product of the Mississippi State University Engineering Research Center. It contains many geometry definition and structured grid generation capabilities. These capabilities are interactively accessible and the resulting geometry and/or grid can be interactively visualized. The code is portable and was installed on both an SGI workstation and a Linux workstation for use by the CFD On-Site Lead in user support.

6.4.2 OVERGRID

OVERGRID is a GUI front end to a set of grid generation utilities made up largely by the Chimera Tool Kit. OVERGRID was developed primarily by Dr. William Chan of NASA Ames. It was designed in close connection with OVERFLOW-D, and thus has many utilities that are specialized for OVERFLOW-D grid systems. This program is best used to define grids for problems to be run with OVERFLOW-D, but it can be used for general grid generation tasks and is available for use by all ERDC MSRC users.

6.4.3 OVERFLOW-D

OVERFLOW-D is a CHSSI CFD code that uses Chimera grid technology in combination with an adaptive background Cartesian grid system. It was developed primarily by Dr. Robert Meakin of the U.S. Army Aero Flightdynamics Directorate. Overall, OVERFLOW-D is one of the best CFD codes available for the solution of moving-body problems. Although there is a long history of the use of OVERFLOW-D at ERDC MSRC, the code is now available pre-compiled, under group-controlled access.

6.4.4 SPEEDES

SPEEDES was exposed to the ERDC MSRC users as part of one-day tutorial delivered on March 22, 2001, at ERDC MSRC. Initial installation on ERDC MSRC Origin3000 was accomplished in March/April and is to be continued throughout the summer of 2001 within the extension project. So far, the Metron version SPEEDES 1.0 has been installed since the JSIMS version does not support IRIX. FSU was able to convert JSIMS tutorial samples to the Metron version and install them as well at ERDC MSRC. This way, the FMS users at ERDC MSRC can get an early preview of and insight into the emergent JSIMS version of the system, based on the currently more stable and mature Metron version.

7. User Support and Impact on User Codes

Since the great majority of users of the ERDC MSRC are off-site, the ERDC MSRC PET effort places emphasis on outreach to remote users, as well as to users located on-site at ERDC. Table 3 lists the contacts made with ERDC MSRC users by the ERDC MSRC PET team during Year 5, and Table 2 lists all travel by the ERDC MSRC PET team in connection with the Year 5 effort. A major component of outreach to ERDC MSRC users is the training courses (described in Section 8) conducted by the ERDC MSRC PET team, some of which are conducted at remote user sites and some of which are Web-based. The ERDC MSRC PET Web site, accessible from the ERDC MSRC Web site, is also a major medium for outreach to ERDC MSRC users.

Specific support activities conducted in Year 5 are described in this section, which is organized by individual components of the ERDC MSRC PET effort. There is overlap of effort among these areas.

7.1 CFD: Computational Fluid Dynamics CTA

(ERC - Mississippi State)

Interactions with ERDC MSRC CFD users have been initiated by a variety of means. Telephone, e-mail, and personal visits have all resulted in opportunities for user support, collaborative efforts, training needs, and technology issues. Long discussions were held with various users, and with Drs. Jay Boris and Jere Matty, the DoD CFD CTA leads, during the *HPC User's Group Meeting*, *AIAA* meetings, and an outreach trip to AEDC.

GGLiB (Geometry and Grid Library) and PMAG (Parallel Multi-block Adaptive Grid System), developed at MSU, were transferred to Dr. Robert Nichols (AEDC), ASC MSRC and Ravi Ramamurti (NRL). The modular library of various functionalities and the CFD PET Web site at MSU will be transferred to ERDC MSRC software repository by June 1, 2001.

7.1.1 CHSSI CFD Codes

The exhibition and the special CHSSI CFD session at the *AIAA Aerospace Sciences* meeting in Reno in January was an excellent vehicle for user outreach and technology transfer. The CFD team has provided support for several CHSSI CFD code efforts:

- Bug fixes, *makefile* improvements, and utilities to OVERFLOW-D (Dr. Robert Meakin, U.S. Army AFDD);
- Compilation of the WIND code on the IBM SP (Chris Nelson, AEDC);
- Improvements and parallelization of the NXair and PEGISUE codes using MPI (Bobby Nichols, Sean Fuller, Greg Denny, and Doyle Young, AEDC);

- Porting and validation of the Beggar code on the IBM SP (Magdi Rizk, Jim Brock, AFSEO);

- Guidance and modifications to 6DOF capabilities of OVERFLOW-D for application to a Challenge project (Jubaraj Sahu, ARL).

Assistance and help was provided in porting the CHSSI CFD solver WIND (AEDC, Contact: Chris Nelson), and in running a generalized grid CFD solver (ARL, Contact: Jubraj Sahu) utilized in the Challenge project led by Dr. Jubraj Sahu (ARL). In particular, help was provided in compilation and run validation on the IBM SP platform at ERDC MSRC and modifications to facilitate 6DOF capabilities of OVERFLOW-D essential to support of the Challenge project.

During an outreach trip to AEDC, parallel implementation of the AEDC CFD code NXair (Contact: Robert Nichols, Sean Fuller, and Bill Riner) using MPI was accomplished. The resulting code performs as well as or better than the previous Pthread implementation, with increased applicability and portability.

A collaborative agreement to improve and parallelize the AEDC Chimera grid assembly code PEGISUE has been made. This enhancement will facilitate overlapping unstructured grids and will provide a functional replacement of the current PEGSUS code. The Beggar code (Eglin AFB, ATSEO, Contact: Magdi Rizk) was ported and improvements in the *makefile* system were made to facilitate running on the IBM SP. Beggar was also validated on this platform.

7.2. CSM: Computational Structural Mechanics CTA

(TICAM – Texas, with ERC – Mississippi State)

7.2.1 CTH

Several software modules or programming tools have been developed or upgraded in support of CSM activity. These include:

- Software modules for inclusion of rigid obstacles into CTH;

- Software modules to allow direct extraction of pressure data from CTH (as can be used, for example, in the generation of load curves for input to finite element models of structures);

- Upgrade/enhancements to software for 2:1 block refinement algorithms in CTH;

- Software modules for 2:1 block-adaptive advection in CTH;

- Upgrade/enhancements to software for error indicator computation in CTH;
- Software modules to allow interfacing of CTH data to other visualization packages;
- Numerous enhancements and bug fixes to sections of CTH written by other developers.

The enhancements to CTH performed in this program represent a leap-ahead advancement in the modeling capability for damage to structures. The adaptive mesh refinement capability extends the capability to problems that before could not be run in a timely manner, and enhances the efficiency and accuracy of calculations that can be run today. Together, the rigid obstacle and pressure extraction interfaces allow for coupling CTH results to structural calculations for blast loading with a fidelity level that before was not possible.

7.2.2 Upgrades to Software for Partitioning Unstructured Grids using Space-Filling Curves

Some of the software modules for error indicators are more broadly applicable (with perhaps minor modification) to other PET program analysis components. The software for adaptive refinement and data structure modification is more specific to the application codes in question but the concepts are general. The module for ordering cells and partitioning based on Space-Filling Curves is written in C++ and has general applicability.

7.2.3 Upgrades to TESTBED for Evaluating Error Indicators and Algorithms in Adaptive Refinement

The TESTBED approach can be applied to other applications and codes with differing physics. It is being tested with scalar transport physics and will be shortly extended to hyperbolic systems with shocks. The integrated effect of these developments on the MSRC is significant since it will provide a new adaptive analysis capability and spearhead similar extensions to the DoD application codes both in CSM and the other PET areas.

7.2.4 SAGE

Rick Weed provided assistance to ERDC Structures Lab personnel in porting and modifying the SAGE hydrocode to the various ERDC MSRC HPC resources. The principal user of SAGE is Bob Britt. The SAGE code went through several upgrades and version changes throughout the year and required continuous support. Dr. Weed's efforts included installing and debugging the code on different platforms, code modification, and the development of a support tool to generate a required data file. The SAGE code is used in explosive effects modeling.

7.2.5 SARA3D

SARA3D is a structural acoustics code developed by BBN Technologies that is used for DoD applications such as submarine design and missile silencing. The NetSolve system developed by PET team member Tennessee is being used to allow the computationally intensive portions of MATLAB-based post-processing for SARA3D to be carried out on HPC machines, while allowing SARA3D users to run the MATLAB programs as usual from their desktop machines.

7.2.6 CSM Challenge Project

Dr. Rick Weed's support for Drs. Bob Bernard and Charlie Berger's Challenge project was initiated after changes in system software on the Origin 2000 introduced errors in a previously working code. Dr. Weed evaluated the two codes used in the project that were coupled using the software package, MDARUN, which Dr. Weed developed in Year 4 PET to support the project- to determine if there was a bug in the software. SGI and ERDC MSRC User Support was unable to identify the problem. Dr. Weed was able to identify the problem and got the code working again. This effort was vital to successful completion of the Challenge project since one of the goals of the project was to demonstrate the scalability and accuracy of the coupled application on more than one MSRC HPC parallel machine.

7.3 CWO: Climate/Weather/Ocean Modeling CTA

(Ohio State)

7.3.1 WAM Wind-Wave Model

The WAM model is used by NAVO to make operational ocean-scale, deep-water wave forecasts for numerous world-wide locations. It is also used at short notice for the rapid deployment support of particular military initiatives. Dr. Bob Jensen of ERDC works closely with NAVO scientists regarding the development of WAM activities and is the main contact for PET activities concerning WAM. In PET Year 5, coupling efforts have continued to involve WAM and the CH3D-SED circulation and sediment transport model within the framework of the COupled MArine Prediction System (COMAPS). In particular, coupling physics and numerics for bottom boundary layer interactions have been upgraded. The most notable impact on WAM predictions will be the more accurate calculation of bottom friction effects.

7.3.2 CH3D-SED Circulation and Sediment Transport Model

The CH3D-SED model is used by ERDC scientists including Drs. Billy Johnson and Jeff Holland. The code predicts marine circulation and sediment transport and is commonly deployed in coastal and estuarine regions. In PET Year 5, activities concerning the CH3D-SED model have been related to the ongoing development of COMAPS, as explained above in the WAM model entry. Modifications to CH3D-SED have focused on using identical sediment transport physics in the SED and WCBL ("Wave-Current Boundary Layer" component of COMAPS) models. This has resulted in improved reference concentration and critical shear stress calculations in SED. The overall upgrade of COMAPS also improves the accuracy of bottom shear stresses used in CH3D-SED.

7.4 EQM: Environmental Quality Modeling CTA

(TICAM – Texas)

7.4.1 UTPROJ3D and INLiB

In multiphysics coupling of numerical fluid flow modeling and transport problems, the computed velocity field frequently needs to be projected from one grid to another among different modules. For accurate transport, it is necessary for the velocities to be locally conservative on the transport grid. The parallel version of UTPROJ3D has been used for coupling the hydrodynamics model TABS-MDS with the water quality model CE-QUAL-ICM.

Collaborating with the MSU CFD PET team to develop general interpolation/projection software by integrating UTPROJ3D with INLiB will allow the use of generic grids for both fluid flow and transport. This software package can also be used in a variety of other areas, including CFD applications and EQM/CWO coupling applications.

7.4.2 Hydrodynamic Model ADCIRC

ADCIRC is a finite element shallow-water hydrodynamics flow model. Users of ADCIRC include Jane Smith and Norm Scheffner of ERDC and researchers at NRL-Stennis. ADCIRC has been used for simulation of coastal and estuaries circulation. It has also been used as the hydrodynamic driver in the coupling of surf zone wave and currents for the near-shore region. The EQM team parallelized ADCIRC and supported ADCIRC validation and evaluation. To optimize parallel load balancing, the EQM team applied data domain decomposition and employed the METIS software for mesh partitioning. A speedup of 120X on 128 PEs was achieved in the simulation of the U.S. East Coast.

7.4.3 Hydrodynamic Model CH3D-Z

CH3D-Z is a three-dimensional numerical hydrodynamic model widely used to investigate important physical features of the hydrodynamic process and bathymetry in rivers and coastal areas. CH3D-Z is also used for studying the impact of contaminant releases from unexploded ordnances, navigability of naval shipping lanes, and channel deepening. Another application of CH3D-Z has been coupling with a water quality model to study pollutant releases into the water column during disposal and/or leaching into the water column from bottom sediments. Users inlude Billy Johnson, Ron Heath, and Rao Vermalukonda of ERDC CHL.

Due to the poor performance and impossibility of parallelizing the code with its current alternating direction (ADI) solution method, the EQM team successfully replaced this solution method by a Jacobi conjugate gradient (JCG) solver. One of the main focuses of this project for PET Year 5 was to improve the performance of the code by a 2-D domain decomposition parallelization. The parallelization has proceeded in the following steps:

(1) A preprocessor was written to split the computational domain into subdomains (using METIS), and to split the physical data into subdomain data to be read by each processor.

(2) MPI calls have been added to the code for message-passing purposes.

Step 1 has been completed and Step 2, now in progress, is expected to be complete by the end of summer 2001.

Another approach has been conducted for improving the performance of the code by using the multiblock grid technique. Preliminary results with a four-block grid on four processors of an IBM SMP show a 3.8X speedup for the simulation of Chesapeake Bay, CND Canal, and Delaware Bay.

7.4.5 Coastal Ocean Circulation Model MGPOM

The Princeton Ocean Model (POM) is widely used by the U.S. Navy for coastal ocean circulation simulation. It also has been coupled with atmospheric and sediment transport models to provide DoD users with an ocean forecasting and near-shore prediction environment. Users include NAVO's oceanographers, NRL-Stennis and NRL-Monterey researchers, and FNOC oceanographers. The dual-level parallel version of the Multiblock Grid Princeton Ocean Model (MGPOM) was developed by the EQM team. MPI is used for message passing between block grids, and OpenMP/Pthreads is used as a second-level parallelization within each block grid. The MPI-OpenMP version of the MGPOM code was used for the simulation of the Arabian Gulf. Performance results from this version show a speedup of 57X on the 20-block rectangular grid and 61X speedup on the 42-block curvilinear grid with nearly double the horizontal grid resolution. Performance results of the MPI-Pthreads version for the U.S. West Coast simulation on the 29-block rectangular grid show a speedup of 41X.

A successful use of the FPTHRD package in the MGPOM (Multiblock Princeton Ocean Model) code was made in collaboration with the Rice SPPT PET team. This is detailed in the reports by Clay Breshears and Phu Luong.

7.4.6 Water Quality Model CE-QUAL-ICM, CE-QUAL-ICM/TOXI

CE-QUAL-ICM is a water quality model that has been widely used by EQM researchers at ERDC MSRC and other MSRC and distributed centers. CE-QUAL-ICM is used for evaluation of proposed dredge material disposal sites, such as New York Harbor, and is also used for evaluation of possible releases and transport of contaminants in the upper Chesapeake Bay area.

One of the main goals of this project for PET Year 5 was a scalability study of CE-QUAL-ICM. VAMPIR was used to evaluate message passing and I/O efficiencies. PAPI was also used for evaluating MFLOPs of the code on the Cray T3E. Based upon this information, the MPI message passing routines were rewritten by using asynchronous sends and receives. Results from these modifications show a 30 percent speedup in addition to the 120X speedup from the previous version. Near optimal speedup (linear with the number of processors) has been observed for the parallel version of CE-QUAL-ICM. In particular, these efforts have resulted in researchers doing EQM studies in less than two weeks. EQM studies previously took a year to complete.

The parallel version 1.4 was delivered to Mark Noel of ERDC in July 2000. The EQM team also worked with Noel to install Carl Cerco's (ERDC) new modifications to the parallel version.

The implementation of the prototype version of CE-QUAL-ICM, which uses MPI-2 style parallel I/O, has been completed for the Cray T3E platform at ERDC. The migration of the parallel I/O version to other platforms, such as Origin 3000 and IBM SMP, is now under-way. Benchmark comparisons of the relative performance of the parallel version 1.4 with the parallel I/O in progress.

Victor Parr at TICAM is also working on CE-QUAL-ICM. The code performs computation using a large number of arrays with the parallel version distributing the arrays in an irregular fashion. These arrays also contain a high percentage of ghost cells (typically 20-35 percent). Typical production level executions perform 10-year simulations. The current solution has each process write results to separate files. This is followed by a post-processing step that must re-read all the output data, re-organize the data, and write the data to a single final output file. A solution that does not require this post-processing step is desired.

7.4.7 LBMPI

LBMPI is a Contaminant Dispersion model EQM challenge code being used by Robert Maier at the Army HPC Research Center (AHPCRC). The code performs computation using what are conceptually four three-dimensional arrays. In practice, however, the four 3-dimensional arrays are stored as a single four-dimensional array. This is done to achieve a better cache-hit ratio. Each of the three-dimensional arrays consists of interior resident cells as well as a layer of ghost cells. The application uses a block-block data distribution. This code is experiencing a severe I/O bottleneck. Running on an IBM SP2 using 512 processors, a typical run requires approximately 12 hours of compute time and an additional 12 hours of I/O time. The traditional Unix-style I/O calls in LBMPI were replaced with parallel I/O calls using the MPI-I/O extensions. This resulted in an I/O speedup of 92X when running on 32 processors.

7.5 Forces Modeling and Simulation/C4I CTA

(Syracuse)

No specific work on user codes was conducted by PET FMS in Year 5, but a potential SPEEDES user was identified at ERDC during the training session. The user was trying to explore the Metron version of the system and had problems with understanding its relation to JSIMS and the status of the software - hence the tutorial and insight into the SPEEDES status were of direct help in clarifying these ambiguities. It turns out that the FMS users today are looking again for a new stable and sustainable M&S platform to be used as a base for their application codes. ModSAF is no longer a viable candidate for such a core system due to its slow transition from DIS to HLA. SPEEDES/JSIMS is now being evaluated as a potential candidate for such a new base platform. It is believed that SPEEDES has much potential, and that this system, when backed by JSIMS, might indeed become a new DoD-wide standard for M&S. SPEEDES offers a sophisticated HPC engine for object-oriented (C++), event-driven (logical time) simulations. It uses the Breathing Time Warp algorithm to manage simulation state rollback and to assure stability and to optimize speedup. It is state-of-the-art parallel simulation technology of relevance for Forces Modeling and Simulation, capable of processing millions of dynamic interacting entities in a wide range of time scales and simulation parameters. It is intended to continue the interaction with ERDC FMS users initiated during the SPEEDES tutorial session and to explore possible joint projects requiring further assistance with hands-on software engineering in the SPEEDES programming environment.

8. User Training

The ERDC MSRC PET training program encompasses a broad range of activities and topics, but the main emphasis is on training directed toward specific high performance computing (HPC) architectures and those Computational Technology Areas (CTAs) supported by the ERDC MSRC. In Year 5, there were training courses on all three ERDC MSRC platforms: the SGI Origin 3000, the Cray T3E, and the IBM Power3 SMP. These training courses are a quick, cost-effective means of getting new users up and running at the ERDC MSRC. The Ohio Supercomputer Center (OSC) continues to be the major supplier of PET training in this area.

8.1 Training Curriculum

PET training is designed to assist the DoD scientists and engineers in efficiently using the present and future HPC hardware acquired through the High Performance Computing Modernization Program (HPCMP). The training curriculum on the ERDC MSRC PET Web site is a living document with new topics continually being added to keep up with the fast pace of research and development in the field of computational science and engineering. The curriculum contains courses in the following general categories:

- Parallel programming
- Architecture and software specific topics
- Visualization and performance
- CTA targeted classes, workshops, and forums

8.2 Web-Based Training

In Year 5, only one training course was broadcast over the Internet using Tango. The Tango system was phased out early in the contract year in favor of Webcasts utilizing the Polycom Stream Station. The Webcast lacks the two-way communication of Tango, but tends to be more reliable and easier to use by both instructor and students. Of the three courses broadcast with the Stream Station, two were taught by instructors from OSC. OSC was involved from the beginning of the PET program with MBONE and Tango and continues to collaborate with the on-site training team on the investigation of new technology for remote training and distance education.

This year brought to a conclusion the PET team's three year experiment with the Tango Interactive collaboratory system of Syracuse. During the Spring 2000 semester, the distance education course "Computational Science for Simulation Applications" was delivered by Geoffrey Fox (formerly of Syracuse) from Florida State University to students at Jackson State University, Morgan State University, Naval Oceanographic Office (NAVO), Naval Research Laboratory (NRL), and the ERDC MSRC. ERDC students received three semester hours of graduate credit from Mississippi State University through the auspices of the ERDC Graduate Institute.

8.3 Training Courses and Material

Training material is available for most courses and selected courses are recorded on VHS tapes. Information on availability of material and tapes may be obtained from the ERDC MSRC Customer Assistance Center by e-mail at info-hpc@wes.hpc.mil or by phone at 601-634-4400 (option 1) or 1-800-500-HPCC. Descriptions for all training courses offered in Year 5 are available on the Web at
http://www.wes.hpc.mil/training/prevcourses/previous.htm.

8.4 Training at Professional Meetings

The ERDC MSRC PET team was active in teaching tutorials at professional meetings. These events were sponsored by the conference organizer and disseminated knowledge not only to the ERDC MSRC users, but also to the larger DoD HPC user community. Dr. Clay Breshears and Dr. Henry Gabb of the PET on-site team taught a tutorial on "Concurrent Programming with Pthreads" at the *DoD HPCMP Users Group Conference* in Albuquerque on June 5, 2000. At the same conference, Dr. Breshears and PET personnel from the Army Research Laboratory (ARL) and the Aeronautical Systems Center (ASC) taught a tutorial entitled "Tools and Techniques for OpenMP, MPI, and Mixed OpenMP and MPI Parallel Programming." Dr. Graham Carey, University CSM Lead at the University of Texas at Austin, delivered a short course on "Adaptive Mesh Generation" at the *9th International Meshing Roundtable* in New Orleans on Oct. 2, 2000.

8.5 Seminars

The ERDC MSRC PET program offers seminars on an irregular basis. These are presentations by experts in their field and are designed to introduce the ERDC MSRC users to current research topics in HPC. The following is a list of seminar presentations during Year 5.

- "Description and Applications of the FEFLO Solver for Solution of the Unsteady Navier-Stokes Equations," Ravi Ramamurti, Naval Research Laboratory, Sept. 12, 2000:

- "Emerging Standards for Training and Education from the DoD and the IMS Consortium," Geoffrey C. Fox, Florida State University, Sept. 18, 2000;

- "Using MPI-I/O," David Cronk, University of Tennessee, Knoxville, Oct. 4, 2000;

- “Recent Developments in Research on Adaptive and Unstructured Grids,” Graham Carey, University of Texas at Austin, Oct. 6, 2000;

- “Parallel Adaptive Algorithms and Software Frameworks for DoD Challenge Class Applications,” Robert T. McLay, University of Texas at Austin, Jan. 10, 2001.

9. HBCU/MI (MSI) Enhancement Program

For Year 5 of the ERDC MSRC PET component of the DoD HPCMP, the Historically Black Colleges and Universities/Minority Institutions (HBCU/MI) team – Minority-Serving Institutions (MSIs) - consisted of Jackson State University, Clark Atlanta University, and Texas A&M University-Kingsville. Dr. Willie Brown of Jackson State was the overall HBCU/MI University Lead for ERDC MSRC PET. This section describes how these institutions participated in PET initiatives at the ERDC MSRC during the fifth year of the program, and how the institutions were enhanced by their involvement. Training courses and seminars conducted by the ERDC MSRC PET team at HBCU/MIs are listed in Table 6.

As the lead university for ERDC MSRC PET, JSU is charged with developing and implementing strategies that allow a two-way exchange between the DoD and HBCU/MI communities. On one hand, minorities are tremendously under represented in the Computational Technology Areas (CTAs) and other HPC efforts within the DoD. On the other hand, the existing pool of talent available to address current and future DoD challenges, using HPC technologies, is limited and decreasing. The PET program provides the DoD with an opportunity to identify and develop new sources of scientific, high-tech, and management personnel. In the opposite direction, PET also affords faculty, staff, and students at HBCU/MIs an opportunity to acquire scientific and HPC-related skills and expertise through interaction with DoD scientists and researchers. JSU's mission is to maximize mutual benefit for both sides by helping to create and maintain pathways between the ERDC MSRC and the HBCU/MI team. Adequate access to HPC facilities and other information technology resources is critical to HBCU/MI participation in this endeavor.

9.1 Jackson State University

JSU is the lead Historically Black College/University (HBCU) for ERDC MSRC PET. JSU's primary mission is to identify and make available to the ERDC MSRC high performance computing (HPC) capabilities and expertise at targeted HBCU/MIs, as well as opportunities for HPC training and capability development/enhancement.

During Year 5, the JSU support team for ERDC MSRC PET, in support of its HBCU/MI mission, was placed under core support. Mr. Chuck Patrick, Scientific Visualization Specialist for JSU, collaborated with ERDC and provided continued scientific visualization support, training, and workshops to faculty, staff, and students. Mr. Patrick conducted several training workshops at JSU in the areas of graphics, animation, and visualization. Training and workshops were provided using software for Maya 3, Advanced Visualization Systems, and Ensight Gold. The training consisted of a series of instructions and hands-on training. All students were introduced and trained on how to operate the SGI machines, techniques, and software.

Tim Ward, the JSU Network Training Specialist, provided technical support to faculty, staff, and students. His duties include any activities involving distance education, such as setting up the lab to receive and send classes via the Internet.

In support of its HBCU/MI mission, JSU hosted the fourth annual High Perfomance Computing Summer Institute on June 12-23, 2000. At the institute, presenters from ERDC and Mississippi State introduced 19 students from seven HBCUs to HPC in general and to the Computational Technology Areas (CTAs) supported at the ERDC MSRC. Students from Mississippi Valley State University, Xavier University in Louisiana, Rusk College, Langston University, Tuskegee University, Dillard University and Jackson State University. As a result of a very successful HPC Summer Institute 2000, students who attended the institute are continuing to e-mail, write, call and communicate with Jackson State. Students impacted by the opportunity to attend the Summer Institute 2000 gained a wide range of knowledge, improved academic performance at their own institutions, and made several career choices centered on high performance computing and DoD.

9.2 Clark Atlanta University

Four minority students participated in both training and research activities offered by Dr. Aliabadi at CAU. All of them have been partially supported through the ERDC MSRC PET program.

- Bruce Zellars (Graduated), Male, African-American, Engineering (Mechanical) at CAU;
- Adetola Abatan (Graduated), Female, African-American, Engineering (Chemical) at CAU;
- James Davis (Junior), Male, African-American, Engineering (Mechanical) at CAU;
- Nayo Morgan (Junior), Female, Jamaican, Engineering (Mechanical) at CAU.

Zellers and Abatan have graduated with bachelor of science degrees in engineering from Clark Atlanta University. Abatan will attend the Ph.D. program at Georgia Institute of Technology in chemical engineering, and Zellars will attend the Ph.D. program at Georgia Institute of Technology in mechanical engineering.

Clark Atlanta also participated in the support of the CFD and CSM CTAs in ERDC MSRC PET in Year 5, as has been described in Section 5.

Richard Anderson completed his second year as a Summer Intern at ERDC MSRC. Richard worked with the on-site training staff and Geoffrey Fox of FSU on an investigation of currently available web conferencing services for delivering distance education and training. He will graduate with a bachelor's degree in computer science from Clark Atlanta University in May 2001.

9.3 Texas A&M – Kingsville

Dr. Thomas L. McGehee, a hydrogeologist and low temperature geochemist in the Department of Geosciences, worked with the Groundwater Technical Support Team during the summer to assist in the development of Parallel FEMWATER in relation to EQM. He also supervised the Parallel FEMWATER visualization project at Texas A&M University-Kingsville. Dr. Michael A. McAdams, a GIS specialist in the Department of Geosciences, supervised two graduate students in the Parallel FEMWATER data management project and provided an overall vision for the linking of HDF5 and Ensight. He also coordinated cooperative efforts between the team and the HDF5 division of the National Center for Supercomputing Applications. This effort is described in Section 5.

The students at Texas A&M University-Kingsville have benefited immensely from PET support through the enhancement of computing software and facilities, enhancement of existing courses, faculty enhancement, supported masters theses, and enhancement of the Applied Groundwater Modeling class.

10. Journal Papers, Presentations, and Reports

10.1 ERDC MSRC PET Technical Reports

01-28 ***Adaptive Mesh Technology, Mesh Improvement and Algorithms for Hypervelocity Impact and Penetration Analysis***, Graham F. Carey, J. Tinsley Oden

01-27 ***A Prototype File Protocol for Application Datasets Based On HDF***, Kent E. Eschenberg, Mike Folk

01-26 ***Comparison of Multiblock Grid and Domain Decomposition in Coastal Ocean Circulation Modeling***, Phu Luong, Clay P. Breshears, Le N. Ly

01-25 ***Review of A Priori Error Estimates for Discontinuous Galerkin Methods***, S. Prudhomme, F. Pascal, J. T. Oden, A. Romkes

01-24 ***Adaptive Mesh Refinement in CTH: Implementation of Block-adaptive Multi-material Refinement and Advection Algorithms***, David L. Littlefield, J. Tinsley Oden, Graham F. Carey

01-23 ***SPEEDES Installation and Training at ERDC MSRC***, Wojtek Furmanski

01-22 ***Improving Parallel Performance for Environmental Quality Models***, Victor J. Parr, Mary F. Wheeler

01-21 ***Ubiquitous Access for Computational Science and Education***, Geoffrey Fox

01-20 ***Architecture and Implementation of a Collaborative Computing and Education Portal***, Geoffrey Fox

01-19 ***Audio Video Conferencing***, Geoffrey Fox, Gurhan Gunduz and Ahmet Uyar

01-18 ***Computational Science and Information Technology: Distance Education and Training***, Geoffrey Fox

01-17 ***Metacomputing Support for the SARA3D Structural Acoustics Application***, Shirley Moore, Dorian Arnold, David Cronk

01-16 ***Enhancement, Evaluation, and Application of a Coupled Wave-Current-Sediment Model Model for Nearshore and Tributary Plume Predictions***, D. J. S. Welsh, K. W. Bedford, Y. Guo, P. Sadayappan

01-15 ***CFDTool: A Web-based Training Tool for CFD***, Roy P. Koomullil, Bharat K. Soni

01-14 ***Improvements in Parallel Chimera Grid Assembly***, Nathan C. Prewitt, Davy M. Belk, Wei Shyy

01-13 ***A Full 2-D Parallel Implementation of CH3D-Z***, Clint Dawson, Victor Parr

01-12 ***Library of Grid Interpolation Modules (INLib)***, S. Gopalsamy, Bharat K. Soni

01-11 ***A Discontinuous Galerkin Discretization for the Mass Conservation Equation in the CE-QUAL-ICM Code***, Krzysztof Bana, Mary F. Wheeler

01-10 ***Development of Parallel 3D Locally Conservative Projection Codes for Reduction of Local Mass***, Mary F. Wheeler, Clint Dawson, Victor J. Parr, Eleanor Jenkins, Jichun Li

01-09 ***Developing Multi-Threaded Fortran Applications Using the PARSA™ Software Development Environment***, Jeff Marquis, Geoffrey Wossum

01-08 ***Visualization for EQM***, Alan M. Shih, M. Pauline Baker

01-07 ***Parallel I/O for EQM Applications***, David Cronk, Graham Fagg, Shirley Moore, Victor Parr

01-06 ***Parallel Finite Element Simulation of Waves Interacting with Ships in Motion***, Shahrouz Aliabadi, Andrew Johnson, Bruce Zellars, Charlie Berger, Jane Smith

01-05 ***Performance Comparison of SGI Origin 2800 and SGI Origin 3800 on Application Codes***, Jeff Hensley

01-04 ***Fortran 77 to Fortran 90 Source Code Conversion and Maintenance Tools***, Richard Weed

01-03 ***Programming Environment and Training (PET) Core Support and Focused Efforts for the period 27 March 2001 through 30 September 2001***

01-02 ***2000 ERDC MSRC PET Training Activities***, Wayne Mastin

01-01 ***Emulating Co-Array Fortran with Pthreads***, Richard J. Hanson, Stephen F. Wornom

00-38 ***The Effect of Wave Propagation Scheme on SWAN Near-shore Wave Predictions***, Stephen F. Wornom, David J.S. Welsh, Keith W. Bedford

00-37 ***On Coupling the SWAN and WAM Wave Models for Accurate Near-shore Wave Predictions***, Stephen F. Wornom, David J.S. Welsh, Keith W. Bedford

00-36 ***Analysis of HPC Usage: ERDC MSRC***, Daniel Duffy

00-35 ***Using OpenMP and Threaded Libraries to Parallelize Scientific Applications***, Daniel Duffy

00-34 ***Tools for Understanding Program Performance***, John Mellor-Crummey

00-33 ***Comparison of OpenMP and Pthreads within a Coastal Ocean Circulation Model Code***, Clay P. Breshears, Phu Luong

00-32 ***Practical Experiences with the Fortran Pthreads API***, Clay P. Breshears, Phu Luong

00-31 ***The Effect of the Wave Propagation Scheme on Near-shore Wave Predictions***, Stephen F. Wornom, David J.S. Welsh, Keith W. Bedford

10.2 CFD

10.2.1 Books and Book Chapters

- **Numerical Grid Generation in Computational Field Simulations**. Proceedings of the *7th International Conference on Grid Generation*, B.K. Soni, J. Hauser, J.F. Thompson, and P.R. Eiseman (editors). International Society of Grid Generation (ISGG), Mississippi State University, September 2000.

- Prewitt, N.C., Belk, D.M., Shyy, W., **Parallel Computing of Overset Grids for Aerodynamic Problems with Moving Objects**, *Progress in the Aerospace Sciences*, Vol. 36 (2000), pp. 117-172.

10.2.2 Journals

- Soni, B.K. **Grid Generation: Past, Present and Future**, *Journal of Applied Numerical Mathematics,* Vol. 32, Issue 4, pp. 261-269, April 2000.

- Kim, S. and Soni, B.K., **Steady 3D Incompressible Flow Analysis for the Simplified Train-Tunnel Interaction**, *Computer Assisted Mechanics and Engineering Sciences,* 7:23-37, 2000.

- Soni, B.K., Koomullil, R.P., Thompson, D.S., and Thornburg, H., **Solution Adaptive Grid Strategies Based on Point Redistribution**, *Comput. Methods Appl. Mech. Engrg.* 189 (2000) 1183-1204.

- Prewitt, N.C., Belk, D.M., and Shyy, W., **Parallel Grid Assembly Within the Beggar Code**, *ISGG Electronic Journal of Grid Generation*, Mississippi State University.

- Aliabadi, S., Shujaee, S., **Two-Fluid Flow Simulations Using Parallel Finite Element Method**, accepted for publication in the *Journal of the Society for Computer Simulation International*.

- Aliabadi, S. and Tezduyar, T., **Stabilized-Finite-Element/Interface-Capturing Technique for Parallel Computation of Unsteady Flows with Interfaces**, *Computer Methods in Applied Mechanics and Engineering*, 190 (2000) 243-261.

- Tezduyar, T. and Aliabadi, S., **EDICT for 3D Computation of Two-Fluid Interfaces**, *Computer Methods in Applied Mechanics and Engineering,* 190 (2000) 403-410.

- Aliabadi, S., Johnson, A., Zellars, B., Abatan, A., and Berger, C., **Parallel Simulation of Flows in Open Channels**, accepted for publication in the *Journal of Future Generation Computer Systems*.

- Aliabadi, S., Johnson, A., and Abedi, J., **Comparison of Finite Element and Pendulum Models for Simulation of Sloshing**, submitted to *Computers and Fluids.*

- Aliabadi, S., Johnson, A., Abatan, A., Abedi, J., Yeboah, Y., and Bota, K., **Stabilized Finite Element Formulation of Buoyancy Driven Incompressible Flows**, submitted to *Communications in Numerical Methods in Engineering.*

- Aliabadi, S., Johnson, A., Zellars, B., Berger, C., and Smith, J., **Parallel Simulation of Waves Interacting with Ship in Motion**, submitted to the *Journal of Applied Ocean Research*.

10.2.3 Proceedings

- Soni, B., Thompson, D., Koomullil, R., and Thornburg, H., **GGTK: A Tool Kit for Static and Dynamic Geometry-Grid Generation and Adaptation**, AIAA 2001-1164, Invited Paper, *39th Aerospace Sciences Meeting*, Reno, Nevada, Jan. 8-11, 2001.

- Soni, B., Hur, J., and Collins, E., **Parametric Grid Generation Applicable to Design Optimization of Centrifugal Compressor Configurations**, AIAA 2000-4862, *8th AIAA/NASA/USAF/ISSMO Symposium on Multidisciplinary Analysis and Optimization*, Long Beach, Calif., Sept. 6-8, 2000.

- Thompson, D., Chalasani, S., and Soni, B.K., **Generation of Volume Meshes by Extrusion from Surface Meshes of Arbitrary Topology**, Proceedings of the *9th International Meshing Roundtable*, New Orleans, La., pp. 385-393, 2000.

- Thompson, D., Chalasani, S., and Soni, B.K., **Generation of Generalized Grids by Extrusion from Surface Meshes of Arbitrary Topology**, Proceedings of the *7th International Conference on Numerical Grid Generation in Computational Field Simulations*, Whistler, B.C., pp. 437-446, 2000.

- Thompson, D. and Soni, B., **Semi-structured Grid Generation in Three Dimensions using a Parabolic Marching Scheme**, AIAA Paper No. 2000-1004, *38th AIAA Aerospace Sciences Meeting*, Reno, Nevada, Jan. 10-14, 2000.

- Soni, B.K., **Synthesis of CFS Environment**, *SIMAI 2000 Conference*, June 5-9, 2000, Ischia, Italy.

- Prewitt, N.C., **Improvements in Grid Assembly for the Beggar Code**, *5th Sym Overset Grids & Solution Technology*, Davis, Calif., August 2000.

- Craciun, G., Thompson, D., Machiraju, R., and Jiang, M., **A Framework for Filter Design Emphasizing Multiscale Feature Preservation**, Proceedings of the *AHPCRC and CASC/LLNL Third Workshop on Mining Scientific Datasets*, pp. 105-111, 2001.

- Choo, Y., Vickerman, M., Lee, K., and Thompson, D., **Geometry Modeling and Grid Generation for Icing Effects and Ice Accretion** Simulations on Airfoils, Proceedings of the *7th International Conference on Numerical Grid Generation in Computational Field Simulations*, Whistler, B.C., pp. 1061-1070, 2000.

- Soni, B., Thompson, D., and Koomullil, R., **Iced Airfoil Simulation using Generalized Grids**, presented at the *16th IMACS World Congress 2000 on Scientific Computation, Applied Mathematics and Simulation*, Lausanne, Switzerland, 2000.

- Nakshatrala, B., Machiraju, R., and Thompson, D., **Exploration and Visualization of Large Datasets**, presented at the *Dagstuhl 2000 Workshop on Scientific Visualization*, Wadern, Germany, 2000.

- Aliabadi, S., Johnson, A., Zellars, B., Abatan, A., and Berger, C., **Parallel Simulation of Flows in Open Channels at Super-Critical Condition Using Finite Element Method**, Abstracts of the *International Conference, Finite Elements in Flow Problems 2000*, University of Texas, Austin, April 30-May 4, 2000.

- Johnson, A., and Aliabadi, S., **Application of Automatic Mesh Generation and Mesh Multiplication Techniques to Very Large Scale Free-Surface Flow Simulations**, Proceedings of the *7th International Conference on Numerical Grid Generation in Computational Field Simulations,* Whistler, British Columbia, Canada, Sept. 25-28, 2000.

- Aliabadi, S. and Johnson, A., **Large-Scale Parallel Simulation of Free-Surface Flow Applications**, Proceedings of the *21st Latin American Congress on Computational Methods in Engineering, Cilamce 2000, Institute of Pure and Applied Mathematics,* Rio de Janeiro, Brazil, Dec. 6-8, 2000.

- Aliabadi, S., Johnson, A., Berger, C., Smith, J., Zellars, B., and Abatan, A., **High Performance Computing in Coastal and Hydraulic Applications**, Proceedings of the *2001 International Parallel and Distributed Processing Symposium*, San Francisco, April 23-27, 2001.

10.2.4 Presentations

- Soni, B. K., Multidisciplinary Simulation and Synthesis, Presentation given at Sandia National Lab (12/00), Boeing Co. (2/01), CIRA, Italy (06/00), JPL (11/00), University of Alabama A&M (2/01), Clark Atlanta University (06/00)

- Soni, B. K., **Geometry and Grid Generation: State-of-the-art, State-of-the-practice**, ERDC MSRC CFD-Day, ASC CFD-Day and ARL CFD-Day.

- Prewitt, N.C., **Overview of Chimera Methods**, CFD Day at ERDC MSRC.

- Prewitt, N.C., **Overview of Chimera Tools**, CFD User's Forum at ASC.

- Aliabadi, S., **Remote Simulation and Visualization of Free-Surface Flow Problems.** *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 5-8, 2000.

- Aliabadi, S., **Parallel Simulation of Free-Surface Flow Problems.** Department of Physics, Clark Atlanta University, Atlanta, Ga., March 2, 2000.

- Aliabadi, S., **Advanced Educational and Computational Technology in Fluid Mechanics.** ARL Review Program, Clark Atlanta University, Atlanta, Ga., April 28, 2000.

- Aliabadi, S., **High Performance Computing for Undergraduates**. Army High Performance Computing Center, University of Minnesota, Minneapolis, Minn., July 13, 2000.

- Aliabadi, S., **New Challenges in Large-Scale CFD Applications**. Army Research Lab, Aberdeen Proving Ground, Md., Oct. 19, 2000.

10.2.5 Reports

- Thompson, D. S., and Soni, B. K., **ICEG2D-An Integrated Software Package for Automated Prediction of Flow Fields for Single-Element Airfoils With Ice Accretion**, NASA/CR-2000-209914

10.3 CSM

10.3.1 Journals

- Carey, G.F., Bicken, G., Carey, V., Berger, C., Sanchez, J., **Locally Constrained Projections**, *Int'l J. for Num. Methods in Engineering*, 50, 549-577, 2001.

- Prudhomme, S., Pascal, F., Oden J., and Romkes, A., ***A priori* Error Estimate for the Baumann-Oden Version of the Discontinuous Galerkin Method**, Accepted, *C.R. Acad. Sci. I, Numer. Anal.*, March 2001.

10.3.2 Proceedings

- Littlefield, D.L., Oden, J., and Carey, G., **Simulation of Hypervelocity Impact Using a Block-Adaptive, Eulerian Impact Mechanics Code**, *HPC2000*, Washington, D.C., April 16-20, 2000.

10.3.3 Presentations

- McLay, R., Prudhomme, S., Carey, G., and Oden, J., **A Platform for Testing Error Indicators in Hypervelocity Impact Problems**, *DoD HPCMP Users Group Conference,* Albuquerque, N. Mexico, June 5-9, 2000.

- Littlefield, D., Oden, J., and Carey, G., **Adaptive Mesh Refinement in CTH: Implementation of Block-Adaptive Multi-material Refinement and Advection Algorithms**, *DoD HPCMP Users Group Conference,* Albuquerque, N. Mexico, June 5-9, 2000.

- Pehlivanov, A., Patra, A., Carey, G., Littlefield, D., and Oden, J., **Error and Shape Quality Indicators for Adaptive Refinement of Deforming Finite Elements**, *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 5-9, 2000.

- Pehlivanov, A., Carey, G., and Iqbal, S., **Studies of Grid Partitioning Algorithms**, *Finite Elements in Flow Problems 2000*, Thompson Conference Center, the University of Texas at Austin, April 30-May 4, 2000.

- McLay, R., Prudhomme, S., Carey, G., Oden, J., **A Platform for Testing Error Indicators in Hypervelocity Impact Problems,** *Finite Elements in Flow Problems 2000*, Thompson Conference Center, the University of Texas at Austin, April 30-May 4, 2000.

- Carey, G., **Finite Element Methodology and Application in Engineering, i**nvited talk at University of Western Australia, Aug. 3, 2000.

- Carey, G., **Modeling in Engineering Analysis and Computation,** Applied Mathematics Department Lecture, University of Western Australia, Aug. 2000.

- Carey, G., **Some Aspects of Finite Element Modeling and Superconvergence in Applied Mathematics,** Seminar, Mathematics Department, University of Western Australia, Aug. 2000.

- Carey, G., Invited Lecture, **Adaptive Grids**, Adaptive Meshing Shortcourse Lecture, prior to *International Meshing Roundtable Conference*, New Orleans, La., Oct. 2, 2000.

- Carey, G., **Some Aspects of Adaptive Grids and Parallel Computation**, Seminar to CSM and other attendees of mid-year review, Vicksburg, Miss, Oct. 6, 2000.

- Carey, G. F., **Superconvergent Flux Extraction, Local Conservation and Properties**. Presentation at *Finite Element Circus*, Rutgers, Oct 20-21, 2000.

- Carey, G., Pehlivanov, A., and Iqbal, S., **Performance of Partitioning Metrics and Comments on their Implications for Adaptive Algorithms**, *First SIAM Conference on Computational Science and Engineering*, Washington D.C., Sept. 21-24, 2000.

- Littlefield, D., Oden, J., and Prudhomme, S., **A Posteriori Error Estimation for Highly Nonlinear Impact Problems**, Chicago, Ill., *ICTAM 2000*, Sept. 1, 2000.

- Carey, G., et al, **Theoretical Aspects of Coupled Codes**, Code Coupling Workshop (PET), San Diego, Ca., Jan. 22-24, 2001.

- McLay, R., **Parallel Adaptive Algorithms and Software Frameworks for DoD Class Applications**, Lecture at ERDC MSRC, Jan. 10, 2001.

- Weed, R., **Building Multidisciplinary Applications with MPI**, Poster session presentation at the *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 5-8, 2000.

10.3.4 Reports

- Prudhomme, S., Pascal, F., Oden, J., and Romkes, A., **A Review of A Priori Error Estimation for Discontinuous Galerkin Methods**, TICAM Report 00-27, the University of Texas at Austin, Oct. 2000.

10.3.5 Conferences/Workshops Organized

- Carey, G., Organized Session on PC Cluster Applications at *HPC 2000*, Washington, D.C., April 16-20, 2000.

- Carey, G. and Oden, J., Co-Organized International Conference, *Finite Elements in Flow Problems 2000 Conference*, Thompson Conference Center, the University of Texas at Austin, April 30-May 4, 2000.

10.4 EQM

10.4.1 Journals

- Dawson, C. and Martinez-Canales, M., **A Characteristic-Galerkin Approximation to a System of Shallow Water Equations**, *Numerische Mathematik*, Vol. 86, pp. 239-256, 2000.

- Dawson, C. and Martinez-Canales, M., **Finite Element Approximations to the System of Shallow Water Equations, Part III: On the Treatment of Boundary conditions**, *SIAM J. Numer. Anal*., Vol. 38, pp. 149-159, 2000.

- Dawson, C. and Kirby, R., **High Resolution Schemes for Conservation Laws with Locally Varying Time-Steps**, to appear in *SIAM J. Sci. Comp*.

- Dawson, C. and Proft, J., **A Priori Error Estimates for Interior Penalty Version of the Local Discontinuous Galerkin Method Applied to Transport Equations**, to appear in *Numerical Methods for Partial Differential Equations*.

- Jenkins, E.W., Kees, C.E., Kelley, C.T. and Miller, C.T., **An Aggregation-Based Domain Decomposition Preconditioner for Groundwater Flow**, *SIAM Journal on Scientific Computing*, to appear.

- Li, J. and Wheeler, M.F., **Uniform Convergence and Superconvergence of Mixed Finite Element Methods on Anistropically Refined Grids**. Accepted for publication in *SIAM J. Numer. Anal*.

- Luong, P.V., Breshears, C.P. and Ly, L.N., **Application of Multiblock Grid and Dual-Level Parallelism in Coastal Ocean Circulation Modeling**. *Journal of Applied Mathematical Modeling*, (In Review).

- Luong, P.V., Breshears, C.P. and Ly, L.N., **Comparison of OpenMP and Pthreads within a Coastal Ocean Circulation Model Code**. Special Issue of *Journal of Scientific Programming*. (In Review).

- Riviere, B., Wheeler, M.F. and Banas, K., **Discontinuous Galerkin Method Applied to a Single Phase Flow in Porous Media. Part II**. Accepted for publication in *Computational Geosciences*.

- Riviere, B. and Wheeler, M.F.**, Discontinuous Finite Element Methods for Acoustic and Elastic Wave Problems. Part I**: Semidiscrete Error Estimates. Submitted for publication to *SIAM J. Numer. Anal*.

- Riviere, B. and Wheeler, M.F., ***A Posteriori* Error Estimates and Mesh Adaptation Strategy for Discontinuous Galerkin Methods Applied to Diffusion Problems**. Accepted for publication in *Computers and Mathematics with Applications*.

- Riviere, B. and Wheeler, M.F., **Discontinuous Galerkin Methods for Flow and Transport Problems in Porous Media**. Submitted for publication to *Communications in Numerical Methods in Engineering*.

- Riviere, B., Wheeler, M.F. and Girault, V., ***A Priori* Error Estimates for Finite Element Methods Based on Discontinuous Approximation Spaces for Elliptic Problems**. Accepted for publication in *SIAM J. Numer. Anal*.

- Wheeler, M.F. and Yotov, I., **Multigrid on the Interface for Mortar Mixed Finite Element Methods for Elliptic Problems**. Vista in Domain Decomposition and Parallel Processing in Computational Mechanics, special issue of *Comp. Meth. in Appl. Mech. and Engng*. Vol. 184 (2000), pp. 287-302.

10.4.2 Proceedings

- Dawson, C., Aizinger, V. and Cockburn, B., **The Local Discontinuous Galerkin Method for Contaminant Transport Problems, Discontinuous Galerkin Methods, Theory, Computation and Applications**, *Lecture Notes in Computational Science and Engineering*, B. Cockburn, G. E. Karniadakis and C.W. Shu, eds., Springer, Berlin, pp. 309-314, 2000.

- Dawson, C., Parr, V.J. and Wheeler, M.F., **Issues in Parallel Computation of Flow and Transport in Surface Waters**, Proceedings of the *International Conference on Parallel and Distributed Processing Techniques and Applications*, Vol. 1, pp. 21-27, Las Vegas, Nev., June, 2000.

- Luong, P.V., Breshears, C.P. and Ly, L.N., **Dual-Level Parallelism & Multiblock Grids in Coastal Ocean Circulation Modeling**. In Proceedings of the *13th International Conference on Parallel & Distributed Computing Systems (PDCS-2000)*, pp. 363-366, Las Vegas, Nev., Aug. 2000.

- Riviere, B. and Wheeler, M.F., **A Discontinuous Galerkin Method Applied to Nonlinear Parabolic Equation**s. *Discontinuous Galerkin Methods, Theory, Computation and Applications*, Springer-Heidelberg (2000) pp. 231-246.

- Wheeler, M.F., **Advanced Techniques and Algorithms for Reservoir Simulation, II: The Multiblock Approach in the Integrated Parallel Accurate Reservoir Simulator (IPARS)**. To appear in Proceedings of *IMA Workshop on Natural Resources*.

- McGehee, T.L., Folk, M., McAdams, M.A., Holland, J.P., Jeagrum, P.K., and Reddy, Bhaskar, **FEMWATER123 Data Management and Visualization of Very Large Data Sets**, *MODFLOW 2001 and Other Modeling Odysses Conference*, Colorado School of Mines, Golden Colo., Sept. 11 through 14, 2001.

10.4.3 Presentations

- Dawson, C., **What does water know about mathematics** . SIAM Student Chapter, Texas Tech University, April 2001.

- Dawson, C., **The Local Discontinuous Galerkin Method for Contaminant Transport and Shallow Water Flows**. Department of Applied Mathematics Colloquium, University of Padova, Italy, March 2001.

- Dawson, C., **Coupling Continuous and Discontinuous Galerkin Methods.** *Workshop on Multiphysics Applications*, ERDC MSRC, Vicksburg, Miss., March 2001.

- Dawson, C., **Discontinuous Galerkin and Time-Split Methods for Reactive Transport Problems**. *Workshop on Solution Methods for Large-Scale Nonlinear Problems*, Pleasanton, Calif., July 2000.

- Dawson, C., **Modeling Flow in Porous Media**. Computational Mathematics Colloquium, Sandia Livermore National Laboratory, Feb. 2001.

- Dawson, C., **The Local Discontinuous Galerkin Method for Contaminant Transport and Shallow Water Flows**. Computational Mathematics Colloquium, University of Houston, Nov. 2000.

- Dawson, C., **The Local Discontinuous Galerkin Finite Element Method**. *Workshop on Reactive Transport*, ERDC MSRC, Vicksburg, Miss., Sept. 2000.

- Dawson, C., **The Local Time Stepping Methods for Transport Problems**. Center for Subsurface Modeling Industrial Affiliates Meeting, Austin, Texas, Oct. 2000.

- Dawson, C., **Discontinuous Galerkin Methods for Contaminant Transport and Shallow Water Problems**. *SIAM Annual Meeting*, Puerto Rico, July 2000.

- Dawson, C., Riviere, B. and Wheeler, M.F., **Discontinuous Galerkin Methods for Flow and Reactive Transport**. *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 2000.

- Jenkins, L., Wheeler, M.F., Vassilevski, Y., Lacroix, S. and Chippada, S., **Solution Techniques for Multiphase Flow in Porous Media**. *Workshop on Multiphysics Application*, ERDC Vicksburg, Miss., March 2001.

- Jenkins, L., **Matrices and the Environment**. Seminar for Math Majors, Trinity University, San Antonio, Texas, February 2001.

- Jenkins, L., **What Do Mathematicians Do?** Presentation to Fifth Grade Math Classes, Austin, Texas, March 2001.

- Jenkins, L., **Newton-Krylov-Schwarz Methods for Hydrology Problems**. *Workshop on Nonlinear Problems*, Pleasanton, Calif., July 2000.

- Jenkins, L., **Aggregation-Based Domain Decomposition Methods for Unsaturated Flow II: Theory and Results**. *SIAM Annual Meeting*, Puerto Rico, July 2000.

- Luong, P.V., **NGLI: Grid Generation and Data Resolution Strategies. Workshop on Multiphysics Application**, ERDC MSRC, Vicksburg, Miss., March 2001.

- Luong, P.V., Breshears, C.P. and Ly, L.N., **Dual-Level Parallelism Improves Load-Balance in Coastal Ocean Modeling**. *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 2000.

- Luong, P.V., Breshears, C.P. and Ly, L.N., **Advantages of Multiblock Curvilinear Grid and Dual-Level Parallelism in Ocean Circulation Modeling**. Poster presentation at *SC2000*, Dallas, Texas, November 2000.

- Wheeler, M.F., **A Distributed Computing Portal for Coupling Multi-physics and Multiple Domains for Environmental Modeling**. NAVOCEANO, Stennis Space Center, Miss., March 2000.

- Wheeler, M.F., **Multiphysics Coupling Environmental Problems**. DoD Symposium, N. Mexico, June 2000.

- Wheeler, M.F., **Locally Conservative Schemes for Modeling Multiphase Flow in Permeable Media**. *SIAM National Meeting*, San Juan, Puerto Rico, July 2000.

- Wheeler, M.F., **Working In A Multidisciplinary Environment**. Association for Women in Mathematics Workshop, *SIAM National Meeting*, San Juan, Puerto Rico, July 2000.

- Wheeler, M.F., **What Does Water Know About Mathematics?** Congressional Lecture Sponsored by American Mathematical Society, Washington, D.C., July 2000.

- Wheeler, M.F., **Coupling of Models for Energy and Environmental Problems**. Plenary Speaker at *First International SIAM Conference on Computational Science*, September 2000.

- Wheeler, M.F.**, Iterative Solvers of the Implicit Parallel Accurate Reservoir Simulator (IPARS)**. Invited speaker at *Solution Methods for Large-Scale Nonlinear Problems*, Pleasanton, Calif., July 2000.

- Wheeler, M.F. and Dawson, C., **Discontinuous Galerkin Methods for Flow and Reactive Transport Diffusion**. *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 2000.

10.4.4 Reports

- Dawson, C., Parr, V.J. and Wheeler, M.F., **Issues in Parallel Computation of Flow and Transport in Surface Waters**. TICAM Report 00-13, May 2000.

- Dawson, C. and Kirby, R., **High Resolution Schemes for Conservation Laws with Locally Varying Time-Steps**. TICAM Report 00-14, May 2000.

- Dawson, C. and Proft, J.**, *A Priori* Error Estimates for Interior Penalty Version of the Local Discontinuous Galerkin Method Applied to Transport Equations**. TICAM Report 00-16, June 2000.

- Jenkins, E.W., Riviere, B. and Wheeler, M.F., ***A Priori* Error Estimate for Mixed Finite Element Approximations of the Acoustic Wave Equation**. TICAM Report 01-09, April 2001.

- Riviere, B., Wheeler, M.F. and Banas, K., ***hp* 3D Flow Simulation with Discontinuous Galerkin Methods**. TICAM Report 00-29, October 2000.

- Riviere, B., Wheeler, M.F., **Optimal Error Estimates for Discontinuous Galerkin Methods Applied to Linear Elasticity Problems**. TICAM Report 00-30, 2000.

- Riviere, B., Wheeler, M.F., Shaw, S. and Whiteman, J.R., **Discontinuous Galerkin Finite Element Methods for Quasi-static Linear Viscoelasticity**. TICAM Report 01-04, 2001.

- Wheeler, M.F. and Riviere, B., **A Discontinuous Galerkin Method Applied to Nonlinear Parabolic Equations**. TICAM Report 99-26, Aug. 2000.

10.5 FMS

None in Year 5.

10.6 Collaboration/Communication

10.6.1 Book Chapters

- Fox, G.C., Hurst, K., Donnellan, A., and Parker, J., **Introducing a New Paradigm for Computational Earth Science – A Web-object-based approach to Earthquake Simulations**, a chapter in AGU monograph on *GeoComplexity and the Physics of Earthquakes* edited by John Rundle, Donald Turcotte and William Klein and published by AGU in 2000, pp. 219-245.

- Fox, G., Furmanski, W., and Haupt, T., **Distributed Systems on the Pragmatic Object Web-Computing with Java and CORBA**, published in *Computational Aerosciences in the 21st Century*, edited by Manuel D. Salas and W. Kyle Anderson, Kluwer Academic Publishing, Dordrecht, The Netherlands, 2000.

10.6.2 Journal

- Fox, G., **From Computational Science to Internetics: Integration of Science with Computer Science**, *Mathematics and Computers in Simulation*, Elsevier, 54 (2000) 295-306.

10.6.3 Proceedings

- Fox, G.C., **Portals and Frameworks for Web-Based Education and Computational Science**, Proceedings of the *Second International Conference on the Practical Application of Java*, Editor Omer Rana, Manchester, England, April 12-14 2000.

10.6.4 Reports

- **Collaboration Tool Survey** is online at: http://aspen.csit.fsu.edu/collabtools/

- Pallickara, S., and Fox, G., **Grid Message Service** http://aspen.csit.fsu.edu/users/shrideep/mspaces/ (Papers and Dissertation thesis)

10.7 SPP Tools

10.7.1 Journals

- Hanson, R.J., Breshears, C., and Gabb, H. **A Fortran Interface to POSIX Threads, submitted to *ACM-Trans. Math. Software***, July 2000. (In review).

- Hanson, R.J. and Wornom, S.F., **Emulating Co-Array Fortran with Pthreads**, submitted to *SIAM Journal on Scientific Computing*, 2001. (In review)

- Browne, S., Dongarra, J., Garner, N., Ho, G., and Mucci. P., **A Portable Programming Interface for Performance Evaluation on Modern Processors**, *International Journal of High-Performance Computing Applications* 14:3, Fall 2000, pp. 189-204.

10.7.2 Proceedings

- Hanson, R.J., Breshears, C., Gabb, H., **Using a Fortran Interface to POSIX Threads**, *The Architecture of Scientific Software*, Eds. R. Boisver, P. Tang, Kluwer Academic Publishers, Boston, Mass. (2001). Presented at *Working Conference 8*, sponsored by IFIP WG2.5, October 2000, Ottawa, Ontario.

- Browne, S., Dongarra, J., Garner, N., London, K., and Mucci, P., **A Scalable Cross-Platform Infrastructure for Application Performance Optimization Using Hardware Counters**, *SC 2000*, Dallas, Texas, November 2000.

- Browne, S. and Cownie, J., **OpenMP Debugging with TotalView**, in Proc. *Workshop on OpenMP Applications and Tools*, San Diego, July 2000.

10.7.3 Presentations

- Breshears, C., Luong, P., **Comparison of OpenMP and Pthreads within a Coastal Ocean Circulation Model Code** at the Workshop on OpenMP Applications and Tools (WOMPAT) in San Diego, July 6-7, 2000.

- Luong, P., Breshears, C., **Hybrid parallelism and Multiblock Grid in Ocean Modeling,** at the *13th International Conference on Parallel and Distributed Computer Systems (PDCS)*, Las Vegas, Nev., August 8-10, 2000.

- Cronk, D., **Metacomputing: An Evaluation of Emerging Systems**, *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 2000.

- Arnold, D., **Secure Remote Access to Numerical Software and Computational Hardware**, *DoD HPCMP Users Group Conference*, Albuquerque, N. Mexico, June 2000.

- Cronk, D., **Using MPI-I/O**, ERDC MSRC, Vicksburg, Miss., August 2000.

10.8 Scientific Visualization

10.8.1 Proceedings

- Stein, R., Shih, A., and Baker, M.P., **Visualization of Water Quality in the Chesapeake Bay**, in proceedings of *IEEE Visualization 2000*, Salt Lake City, Utah, October 8-13, 2000.

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
ERC (Mississippi State) – Leadership					
Joe Thompson, PhD	Mississippi State	At University	Distinguished Professor	50	12

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
ERC (Mississippi State) – CFD					
Bharat Soni, PhD	Mississippi State	At University	Professor	20	6
Nathan Prewitt, PhD	Mississippi State	On-Site	Research Engineer	100	All
Roy Koomullil, PhD	Mississippi State	At University	Research Engineer	40	0
David Thompson, PhD	Mississippi State	At University	Research Engineer	10	0
Sankarappan Gopalsamy, PhD	Mississippi State	At University	Research Engineer	20	1
David O'Gwynn	Mississippi State	At University	Graduate Student	50	4
Eric Collins	Mississippi State	At University	Graduate Student	50	0
Jennifer Collins	Mississippi State	At University	Technical Support	15	0
Ruparani Chittineni	Mississippi State	At University	Graduate Student	25	0
Anne McClain	Mississippi State	At University	Graduate Student	25	1

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
ERC (Mississippi State) – CFD					
Satish Chalasani	**Mississippi State**	**At University**	**Graduate Student**	**10**	**0**
Melissa Stumpe	**Mississippi State**	**At University**	**Graduate Student**	**50**	**0**
Kenneth Fazel	**Mississippi State**	**At University**	**Undergraduate Student**	**50**	**0**
James Tullos	**Mississippi State**	**At University**	**Undergraduate Student**	**50**	**0**

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
TICAM (Texas) & ERC (Mississippi State) -- CSM					
J. Tinsley Oden, PhD	Texas	At University	Professor, Director TICAM Cockrell Family Regents Chair in Engineering #2	3	0
Graham Carey, PhD	Texas	At University	Professor Curran Chair	0	4
Rick Weed, PhD	Mississippi State	On-Site	Research Engineer	100	All
A. Ardelea, PhD	Texas	At University	Post Doctoral Fellow	37	0
D. Littlefield, PhD	Texas	At University	Research Scientist	71	5
R. McLay, PhD	Texas	At University	Research Associate	48	2
A. Pehlivanov, PhD	Texas	At University	Research Associate	0	0
S. Prudhomme, PhD	Texas	At University	Post Doctoral Fellow	23	0
A. Pardhanani, PhD	Texas	At University	Research Associate	18	0
T. Walsh, PhD	Texas	At University	Post Doctoral Fellow	15	0

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
TICAM (Texas) & ERC (Mississippi State) – CSM					
M. Anderson	Texas	At University	Graduate Research Assistant	37	0
J. Bailey	Texas	At University	Graduate Research Assistant	9	0
W. Barth	Texas	At University	Graduate Research Assistant	13	0
P. Bozeman	Texas	At University	Administrative Associate	12	0
M. Brewer	Texas	At University	Graduate Research Assistant	9	0
B. Carnes	Texas	At University	Graduate Research Assistant	41	0
S. Iqbal	Texas	At University	Graduate Research Assistant	9	0
C. Kavouklis	Texas	At University	Graduate Research Assistant	14	0
B. Kirk	Texas	At University	Graduate Research Assistant	31	0
L. Larkey	Texas	At University	Graduate Research Assistant	28	0

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
TICAM (Texas) & ERC (Mississippi State) -- CSM					
T. Miler	Texas	At University	Graduate Research Assistant	11	0
D. Pardo	Texas	At University	Graduate Research Assistant	10	0
A. Romkes	Texas	At University	Graduate Research Assistant	11	0
A. Staelens	Texas	At University	Graduate Research Assistant	20	0
P. Udomjukkavut	Texas	At University	Graduate Research Assistant	9	0
K. Vemaganti	Texas	At University	Graduate Research Assistant	3	0
X. Wang	Texas	At University	Graduate Research Assistant	9	0

Table 1 Technical Support Team Personnel					
Team Member	**Affiliation**	**Location**	**Title**	**% Time**	**Days On-Site**
Ohio State – CWO					
Keith Bedford, PhD	**Ohio State**	**At University**	**Prof. and Chair, Dept. of Civil and Environmental Engineering and Geodetic Science**	**5**	**2**
Ponnuswamy Sadayappan, PhD	**Ohio State**	**At University**	**Professor**	**8.3**	**2**
Stephen Wornom, PhD	**Ohio State**	**On-Site**	**Senior Research Scientist**	**100**	**All**
David Welsh, PhD	**Ohio State**	**At University**	**Senior Research Associate - Engineer**	**100**	**10**
Rong Wang	**Ohio State**	**At University**	**Graduate Student**	**25**	**0**

Table 1 Technical Support Team Personnel					
Team Member	**Affiliation**	**Location**	**Title**	**% Time**	**Days On-Site**
TICAM (Texas) – EQM					
Mary Wheeler, PhD	**Texas**	**At University**	**Professor Ernest and Virginia Cockrell Chair**	**12.5**	**4**
Clint Dawson, PhD	**Texas**	**At University**	**Professor**	**12.5**	**4**
Phu Luong, PhD	**Texas**	**On-Site**	**Research Scientist**	**100**	**All**
Victor Parr, PhD	**Texas**	**At University**	**Research Scientist**	**100**	**2**
Eleanor White Jenkins, PhD	**Texas**	**At University**	**Research Scientist**	**25**	**8**
Krzysztof Banas, PhD	**Texas**	**At University**	**Research Scientist**	**8.5**	**2**
William Wuertz	**Texas**	**At University**	**Staff**	**16.5**	**0**

Table 1 Technical Support Team Personnel					
Team Member	**Affiliation**	**Location**	**Title**	**% Time**	**Days On-Site**
Florida State & NPAC (Syracuse) – FMS & C/C					
Geffory. Fox, PhD	**Florida State**	**At University**	**Professor**	**15**	**3**
O. Balsoy	**Syracuse**	**At University**	**Graduate Student**	**26**	**0**
G. Gunduz	**Syracuse**	**At University**	**Graduate Student**	**44**	**0**
M. Ispirli	**Syracuse**	**At University**	**Graduate Student**	**32**	**0**
J. Kim	**Florida State**	**At University**	**Graduate Student**	**28**	**0**
K. Kim	**Florida State**	**At University**	**Graduate Student**	**27**	**0**
H. Lee	**Florida State**	**At University**	**Graduate Student**	**10**	**0**
S. Lee	**Florida State**	**At University**	**Graduate Student**	**35**	**0**
S. Lim	**Florida State**	**At University**	**Graduate Student**	**10**	**0**
E. Mohamed	**Florida State**	**At University**	**Graduate Student**	**16**	**0**

Table 1 Technical Support Team Personnel					
Team Member	**Affiliation**	**Location**	**Title**	**% Time**	**Days On-Site**
Florida State & NPAC (Syracuse) – FMS & C/C					
S. Oh	**Florida State**	**At University**	**Graduate Student**	**35**	**0**
S. Pallickara	**Syracuse**	**At University**	**Graduate Student**	**40**	**0**
A. Uyar	**Syracuse**	**At University**	**Graduate Student**	**37**	**1.5**
M. Wang	**Syracuse**	**At University**	**Graduate Student**	**26**	**0**

Table 1 Technical Support Team Personnel					
Team Member	**Affiliation**	**Location**	**Title**	**% Time**	**Days On-Site**
NCSA (Illinois) – SV					
Polly Baker, PhD	**Illinois**	**At University**	**Academic Lead**	**5**	**4**
Mike Folk, PhD	**Illinois**	**At University**	**Senior Software Engineer**	**5**	**0**
Alan Shih, PhD	**Illinois**	**At University**	**Research Scientist**	**30**	**0**
Muqun Kent Yang	**Illinois**	**At University**	**Research Assistant**	**30**	**0**
Su Xiangyang	**Illinois**	**At University**	**Graduate Research Assistant**	**50**	**0**

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
CRPC (Rice, Tennessee) SPP Tools					
Clay Breshears, PhD	Rice	On-Site	Research Scientist	100	All (Apr-Aug)
Richard Hanson, PhD	Rice	At University	Research Scientist	50	Half (Sept-Mar)
Shirley Moore, PhD	Tennessee	At University	Associate Director	20	0
Graham Fagg, PhD	Tennessee	At University	Research Assistant Professor	20	0
David Cronk	Tennessee	At University	Research Associate	50	4
Dorian Arnold	Tennessee	At University	Research Associate	10	0

Table 1
Technical Support Team Personnel

Team Member	Affiliation	Location	Title	% Time	Days On-Site
Jackson State University					
Willie G. Brown, Ph.D.	**Jackson State**	**At University**	**VP for Information Technology**	**10**	**20**
Chuck Patrick	**Jackson State**	**At University**	**Scientific Visualization Specialist**	**100**	**5**
Timothy Ward	**Jackson State**	**At University**	**Network Training Specialist**	**25**	**1**
Brenda Rascoe	**Jackson State**	**At University**	**Administrative Assistant**	**50**	**3**

Table 1 Technical Support Team Personnel					
Team Member	**Affiliation**	**Location**	**Title**	**% Time**	**Days On-Site**
Texas A & M University At Kingsfield – EQM					
Thomas Lee McGehee, PhD	**TAMK**	**At University**	**Associate Professor**	**25**	**9**
Michael A. McAdams, PhD	**TAMK**	**At University**	**Assistant Professor**	**20**	**4**
Bhaskar Reddy	**TAMK**	**At University**	**Graduate Student**	**50**	**2**
Pavan Kumar	**TAMK**	**At University**	**Graduate Student**	**50**	**0**
Paul Thareval	**TAMK**	**At University**	**Graduate Student**	**50**	**0**
Hritkik Patel	**TAMK**	**At University**	**Graduate Student**	**50**	**0**
Sonali Deshpande	**TAMK**	**At University**	**Graduate Student**	**50**	**0**

Table 1 Technical Support Team Personnel					
Team Member	**Affiliation**	**Location**	**Title**	**% Time**	**Days On-Site**
Clark Atlanta University – CFD/CSM					
Shahrouz Aliabadi, PhD	**CAU**	**At University**	**Associate Professor**	**30**	**4**
Adetola Abatan	**CAU**	**At University**	**Graduate Student**	**60**	**0**
Bruce Zellars	**CAU**	**At University**	**Graduate Student**	**60**	**0**
James Davis	**CAU**	**At University**	**Graduate Student**	**20**	**0**
Nayo Morgan	**CAU**	**At University**	**Graduate Student**	**70**	**0**

Table 2 **Team Travel**				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
ERC (Mississippi State) – Leadership				
ERDC MSRC	**Mississippi State**	**Thompson**	**7**	**Leadership Discussions**
Washington, DC	**Mississippi State**	**Thompson**	**2**	**Meeting with HPCMO**
Albuquerque, NM	**Mississippi State**	**Thompson**	**5**	**DoD HPCMP Users Group Conference**
Whistler, BC, Canada	**Mississippi State**	**Thompson**	**5**	**7th International Conference on Numerical Grid Generation and Computational Field Simulation**
ERDC MSRC	**Mississippi State**	**Thompson**	**2**	**ERDC MSRC PET Mid-Year Review**
Dallas, TX	**Mississippi State**	**Thompson**	**7**	**Supercomputing 2000**
ERDC MSRC	**Mississippi State**	**Thompson**	**3**	**ERDC MSRC PET Annual Review**

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
ERC (Mississippi State) – CFD				
ERC (MSU)	Mississippi State	Prewitt	1	ERDC MSRC PET Coordination
ERDC MSRC	Mississippi State	Soni	2	ERDC MSRC PET Annual Review
ERC (MSU)	Mississippi State	Prewitt	4	Technology Tracking, Challenge Project Coordination
ARL MSRC	Mississippi State	Soni, Prewitt	2	ARL MSRC PET Mid-Year Review/User Outreach/Collaboration
ERDC MSRC	Mississippi State	Soni	1	CFD Day
Albuquerque, NM	Mississippi State	Prewitt	5	DoD HPCMP Users Group Conference
ERC (MSU)	Mississippi State	Prewitt	2	Technology Tracking, Rick Cozby - VPG
ERDC MSRC	Mississippi State	Soni, Stumpe, McClain	1	Chimera discussion, Structures Lab Visit
Eglin AFB, FL	Mississippi State	Prewitt	1	Site Visit – AFSEO
ERDC MSRC	Mississippi State	O’Gwynn	2	Chimera Focused Effort

Table 2
Team Travel

Destination	Institution	PET Personnel	Duration (Days)	Purpose
ERC (Mississippi State) – CFD				
ERC (MSU)	Mississippi State	Prewitt	2	Training for Mary Jane Graham, Overgrid Demo
Washington, DC	Mississippi State	Soni, Prewitt	1	CFD Users Forum
ERDC MSRC	Mississippi State	Soni	1	FEFLO Seminar
UC Davis	Mississippi State	Prewitt	2	5th Symposium on Overset Grids and Solution Technology
Whistler, BC, Canada	Mississippi State	Soni, Prewitt, E. Collins, J. Collins, Chittineni, Koomullil	5	7th International Conference on Numerical Grid Generation and Computational Field Simulation
New Orleans, LA	Mississippi State	Soni	4	Interaction Meshing Roundtable
Cincinnati, OH	Mississippi State	Soni	2	Visit with Jay Boris, CFD CTA Lead Dr. Ravi Ramamurti, Outreach
ERDC MSRC	Mississippi State	O'Gwynn	1	Chimera Focused Effort
ERC (MSU)	Mississippi State	Prewitt	2	PEGISUE, Collaboration with AEDC
Phillips Laboratory	Mississippi State	Soni	2	Outreach

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
ERC (Mississippi State) – CFD				
Reno, NV	**Mississippi State**	**Soni, Koomullil, and D. Thompson**	**5**	**39th AIAA Aerospace Sciences Meeting**
ERC (MSU)	**Mississippi State**	**Prewitt**	**1**	**Chimera Focused Effort**
ERDC MSRC	**Mississippi State**	**O'Gwynn, Gopalsamy**	**1**	**Chimera and INLib Focused Efforts**
ERC (MSU)	**Mississippi State**	**Prewitt**	**1**	**ERDC MSRC PET Coordination**
ERDC MSRC	**Mississippi State**	**Soni**	**2**	**ERDC MSRC PET Annual Review**
AEDC	**Mississippi State**	**Soni, Prewitt**	**2**	**Site Visit/Meeting with CFD CTA Lead**
ARL MSRC	**Mississippi State**	**Prewitt**	**4**	**CFD++ Class/Challenge Project**

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
TICAM (Texas) & ERC (Mississippi State) – CSM				
Washington, DC	Texas	Littlefield	2	Presentation at Advanced Simulation Technologies Conference
Albuquerque, NM	Texas	Littlefield, McLay, Pehlivanov, Weed	3	Presentations at DoD HPCMP Users Group Conference
Austin, TX	Texas	Patra	15	Collaboration on NRC project
Washington, DC	Texas	Carey	6	Presentation at SIAM Conference
ERDC MSRC	Texas	Carey	2	ERDC MSRC PET Midyear Review
Dallas, TX	Texas	Carey, Littlefield, McLay, Barth	4	Presentation at SC2000 Conference
La Jolla, CA	Texas	Oden Carey	2	ERDC MSRC PET CSM PI Meeting
ERDC MSRC	Texas	McLay	2	Software Frameworks Workshop at ERDC MSRC
San Diego, CA	Texas, MSU	Carey, Littlefield, McLay, Weed	4	Code Coupling Workshop sponsored by ERDC MSRC

Table 2 **Team Travel**				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
TICAM (Texas) & ERC (Mississippi State) – CSM				
ERC (MSU)	**Texas**	**Brewer** **Kavouklis**	**3**	**Meeting with Bharat Soni at Mississippi State**
ERDC MSRC	**Texas**	**Carey** **Littlefield**	**2**	**ERDC MSRC PET Annual review**
ERDC MSRC	**Texas**	**Littlefield**	**1**	**AMR-CTH tutorial**
ERDC MSRC	**Texas**	**Littlefield**	**2**	**ALE Short Course at ERDC MSRC**
Austin, TX	**MSU**	**Weed**	**5**	**Finite Elements in Fluids Conference at U.T. Austin**
State College, PA	**MSU**	**Weed**	**5**	**Modern Protective Structures Short Course at Penn State**

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
Ohio State – CWO				
ERDC MSRC	**Ohio State**	**Welsh**	**3**	**Mesoscale Atmospheric Models workshop**
Washington, DC	**Ohio State**	**Wornom**	**2**	**Advanced Topics in UNIX workshop**
Albuquerque, NM	**Ohio State**	**Wornom Welsh**	**5**	**DoD HPCMP Users Group Meeting**
NAVO MSRC	**Ohio State**	**Wornom**	**1**	**Meet with the CWO DoD Lead, George Heburn, to deliver recent published ERDC MSRC PET**
Ohio State	**Ohio State**	**Wornom**	**2**	**ERDC MSRC PET mid-year review**
ERDC MSRC	**Ohio State**	**Welsh Sadayappan**	**2**	**Met with ERDC CHL scientists Joe Gailani, Jim Clausner, Norm Sheffner, Bob Jensen, and Rebecca Brooks concerning Focused Effort activities**
Dallas, TX	**Ohio State**	**Wornom**	**5**	**SC2000**
ERDC MSRC	**Ohio State**	**Welsh**	**3**	**Introduction to the SWAN Wave Model workshop**
ERDC MSRC	**Ohio State**	**Bedford Welsh**	**2**	**ERDC MSRC PET Annual Review**

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Dates)**	**Purpose**
TICAM (Texas) – EQM				
ERDC MSRC	Texas	Wheeler, Dawson, Jenkins, Banas, Riviere	2	Reactive Transport
ERDC MSRC	Texas	Wheeler, Dawson, Jenkins	3	ERDC MSRC PET Annual Review
NAVO MSRC	Texas	Wheeler, Dawson, Luong	2	Discussed EQM Project
ERC (MSU)	Texas	Wheeler, Dawson, Luong	2	Discussed EQM Projects
ERDC MSRC	Texas	Dawson, Jenkins	2	Multiphysics Workshop
ERDC MSRC	Texas	Jenkins	2	Discussion with EQM Users on ADH
ERDC MSRC	Texas	Parr, Jenkins	2	Discussed UTPROJ3D with MSU CFD and EQM Users
Austin, TX	Texas	Luong	7	Worked with UT-Austin PET Year 5 Projects and Quarterly Reports
San Diego, CA	Texas	Luong	5	Presented Paper at WOMPAT Workshop

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Dates)**	**Purpose**
TICAM (Texas) – EQM				
New Orleans, LA	Texas	Luong	7	Attended SIGGRAPH2000
Las Vegas, NV	Texas	Luong	5	Presented Paper at PDCS Conference
San Diego, CA	Texas	Luong	3	Worked with Dr. Sinkovits at SDSC on Optimization of CH3D-Z code
Austin, TX	Texas	Luong	5	Worked with UT-Austin on Mid Year Review and Proposals for 6 Months Extension
Austin, TX	Texas	Luong	13	Attended Center for SubsurfaceModeling Affiliates Meeting
Dallas, TX	Texas	Luong	6	Presented Poster at SC2000
Austin, TX	Texas	Luong	7	Worked with UT-Austin on Annual Review PET Year 5

Table 2
Team Travel

Destination	Institution	PET Personnel	Duration (Dates)	Purpose
Florida State & NPAC (Syracuse) – FMS & C/C				
Dallas, TX	Florida State	G. Fox	7	SC2000
ERDC MSRC	Florida State	G. Fox	3	ERDC MSRC PET Annual Review
ERDC MSRC	Florida State	G. Fox A. Uyar	1	Presenting Tutorial on Collaboration Systems

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
CRPC (Rice, Tennessee) – SPPT				
University of Tennessee	**Rice**	**Breshears**	**6**	**Prepare for ERDC MSRC and SC2000 Tutorials**
Rice University	**Rice**	**Breshears**	**3**	**Work on Fortran API paper at Rice**
Boulder, CO	**Rice**	**Breshears**	**4**	**Attend Ptools Consortium Conference**
Albuquerque, NM	**Rice**	**Breshears**	**7**	**Presentation at DoD HPCMP User Group Conference**
NAVO MSRC	**Rice**	**Breshears**	**2**	**Give talk at NAVO MSRC**
San Diego, CA	**Rice**	**Breshears**	**5**	**Presentation at WOMPAT 2000 Conference**
Las Vegas, NV	**Rice**	**Breshears**	**6**	**Attend PDCS2000 Conference**
Dayton, OH	**Rice**	**Breshears**	**3**	**Attend MAPINT Conference**
Texas Tech	**Rice**	**Hanson**	**2**	**Give talk at Texas Tech., Computer Science Department, on Fortran API to Pthreads**
Albuquerque, NM	**Rice**	**Hanson**	**5**	**Attend and speak at DoD HPCMP User Group Conference**

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
CRPC (Rice, Tennessee) – SPPT				
ERDC MSRC	**Rice**	**Hanson**	**14**	**On-site support**
ERDC MSRC	**Tennessee**	**Cronk**	**2**	**MPI-I/O Seminar and PET Mid-Year Review**
ERDC MSRC	**Tennessee**	**Cronk**	**2**	**ERDC MSRC PET Annual Review**

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
NCSA (Illinois) – SV				
ERDC MSRC	**Illinois**	**Baker**	**2**	**ERDC MSRC PET Annual Review**

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
Jackson State				
New Brunswick, NJ	Jackson State	Patrick	5	VR 2000 Workshop
ERDC MSRC	Jackson State	Brown Patrick	1	Consultation at ERDC MSRC
ERDC MSRC	Jackson State	Patrick Rascoe	1	ERDC MSRC, Technical Interchange Briefing Workshop
ERC (MSU)	Jackson State	Patrick Rascoe	3	Summer Institute 2000 students at MSU
ERDC MSRC	Jackson State	Patrick Rascoe	1	Summer Institute 2000 students at ERDC
Scottsdale, AR	Jackson State	Patrick	4	Image 2000 Conference
New Orleans, LA	Jackson State	Patrick	6	SIGGRAPH 2000
ERDC MSRC	Jackson State	Rascoe	1	9th Conference on Current Trends In Computational Chemistry
Chicago, IL	Jackson State	Brown	1	Visit Argonne Laboratory/Access Grid Node
ERDC MSRC	Jackson State	Patrick	1	Meeting with ERDC MSRC Scientific Visualization Group

Table 2 Team Travel				
Destination	**Institution**	**PET Personnel**	**Duration (Days)**	**Purpose**
Jackson State				
ERDC MSRC	**Jackson State**	**Patrick**	**1**	**Collaboration at ERDC with Dr. Kent Eschenburg/Visualization Project/Spring Workshop**
Hattiesburg, MS	**Jackson State**	**Rascoe**	**2**	**Creating Futures Through Technology Conference**
ERDC MSRC	**Jackson State**	**Ward**	**1**	**Meeting at ERDC MSRC on Access Grid**

Table 2
Team Travel

Destination	Institution	PET Personnel	Duration (Days)	Purpose
Clark Atlanta				
ERDC MSRC	CAU	Aliabadi	2	Multi-Physics Workshop
San Francisco, CA	CAU	Aliabadi, Abedi	7	Presentation at the 2001 International Parallel and Distributed Processing Symposium
Austin, TX	CAU	Aliabadi, Zellars, Abatan	5	Presentation at the International Conference in Finite Elements in Flow Problems 2000
Albuquerque, NM	CAU	Aliabadi	4	Presentation at the DoD HPCMP Users Group Conference
ERDC MSRC	CAU	Aliabadi	3	ERDC MSRC PET Year End Review
Dallas, TX	CAU	Aliabadi	3	Attended SC2000
Whistler, British Columbia, Canada	CAU	Aliabadi	4	Presenter at the 7th International Conference on Numerical Grid Generation in Computational Field Simulations

Table 2 **Team Travel**				
Destination	**Institution**	**PET Personnel**	**Duration (Dates)**	**Purpose**
Texas A & M – Kingsfield				
ERDC MSRC	**TAMK**	**McAdams**	**2**	**HDF5 Training at ERDC MSRC**
ERDC MSRC	**TAMK**	**McGehee, Reddy**	**2**	**HDF5 Training at ERDC MSRC**
Champaign, IL	**TAMK**	**McAdams, Petel, Reddy**	**4**	**HDF5 Training**
ERDC MSRC	**TAMK**	**McGehee**	**90**	**Work with ERDC MSRC PET Team**
Champaign, IL	**TAMK**	**Reddy**	**5**	**Work with HDF5 Team**
ERDC MSRC	**TAMK**	**McGehee, McAdams**	**3**	**ERDC MSRC PET Annual Review**

Table 3
ERDC MSRC User Contacts

CEWES User	User Site	CTA	ERDC PET Team Member	Mode of Contact	Purpose/Result
CFD					
Steven Standley	AFSEO/Eglin	CFD	Prewitt	Phone/Email/Visit	Beggar Application Support
Magdi Rizk, Steve Ellison, Jim Brock	AFSEO/Eglin	CFD	Prewitt	Phone/Email/Visit	Beggar Development
Joe Keen	AFSEO/Eglin	CFD	Prewitt	Phone/Email/Visit	Parallel Programming Environment
Doug Plotner	MSU/ERC	CFD	Prewitt	Phone/Email/Visit	IBM SP Run Support
Joe Baum	SAIC	CFD	Prewitt	Phone/Email	Challenge Project Coordination
Chris Nelsen	AEDC	CFD	Prewitt	Phone/Email/Visit	Wind Code Port added to IBM SP
Jubraj Sahu	ARL	CFD	Prewitt	Email/Visit	Challenge Project Support
Daniel Lesieutre	Nielson Research	CFD	Prewitt	Phone	Access to Overflow
Bobby Nichols, Sean Fuller, Bill Riner	AEDC	CFD	Prewitt	Phone/Email/Visit	MPI Implementation of NXair
Bobby Nichols, Sean Fuller, Greg Denny, Doyle Young	AEDC	CFD	Prewitt	Phone/Email/Visit	PEGISUE Development

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
CFD					
Balu Sekar	**ASC**	**CFD**	**Prewitt**	**Email/Visit**	**Access to TIGER**
Mary Jane Graham	**ARL/West Point**	**CFD**	**Prewitt**	**Visit**	**Chimera Technology Training**
Ron Schultz	**NRL**	**CFD**	**Prewitt**	**Phone**	**WIND Support**
Charlie Berger, Barry Bunch, Gary Brown	**ERDC CHL, EL**	**CFD**	**Prewitt**	**Visit**	**INLib Demo Project**
Tim Madden	**AF Phillips Lab**	**CFD**	**Soni**	**Visit**	**PMAG-Transfer & acquaintance with grid adaptation Challenge project**
Robert Nichols	**AEDC**	**CFD**	**Soni**	**Visit/Email**	**GGLib & CAGI Demonstration**
Carolyn Kaplan, David Mott, Ingrid Wysong	**NRL, AF Phillips Lab**	**CFD**	**Soni**	**AIAA Aerospace Science Meeting – CHSSI Session/Email**	**Training course requirements in MPI & Geometric-Grid CAGI software**
Norm Suhs	**Redstone Arsenal**	**CFD**	**Soni**	**AIAA Aerospace Science Meeting – CHSSI Session**	**Collaboration in Chimera Technology**

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
CSM					
James Baylot	ERDC SL	CSM	Littlefield	Phone Email	INGRID coupling
James Baylot	ERDC SL	CSM	Littlefield	Visit	AMR-CTH tutorial
James Baylot	ERDC SL	CSM	Littlefield	Visit	ALE class
James Baylot	ERDC SL	CSM	McLay	Visit	Frameworks Workshop
Tommy Bevins	ERDC SL	CSM	Littlefield	Phone Email	Test Problems
Tommy Bevins	ERDC SL	CSM	Littlefield	Visit	AMR-CTH tutorial
Tommy Bevins	ERDC SL	CSM	Littlefield	Visit	ALE class
Steve Akers	ERDC SL	CSM	Littlefield	Visit	ALE class
Steve Akers	ERDC SL	CSM	McLay	Visit	Frameworks Workshop
James O’Daniel	ERDC SL	CSM	Littlefield	Visit	AMR-CTH tutorial

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
CSM					
James O'Daniel	ERDC SL	CSM	McLay	Visit	Frameworks Workshop
James O'Daniel	ERDC SL	CSM	Littlefield	Visit	ALE class
Byron Armstrong	ERDC SL	CSM	Littlefield	Visit	ALE Class
Charlie Berger	ERDC CHL	CSM	McLay	Visit	Frameworks Workshop
Stacy Howington	ERDC CHL	CSM	McLay	Visit	Frameworks Workshop
Raju Namburu	ARL	CSM	Littlefield	Email	AMR enhancements
Kent Kimsey	ARL	CSM	Littlefield	Visit	Armor modeling discussions, AMR-CTH
Steve Schraml	ARL	CSM	Littlefield	Visit	Armor modeling discussions, AMR-CTH
Dan Scheffler	ARL	CSM	Littlefield	Visit	Armor modeling discussions, AMR-CTH

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
CSM					
Dave Kleponis	**ARL**	**CSM**	**Littlefield**	**Visit**	**Armor modeling discussions, AMR-CTH**
Bob Britt	**ERDC SL**	**CSM**	**Weed**	**Visit, Phone, Email**	**Discussions about SAGE code**
Jimmy Baylott	**ERDC SL**	**CSM**	**Weed**	**Visit, Phone, Email**	**Discussions about Code Coupling Workshop**
Robert Hall	**ERDC SL**	**CSM**	**Weed**	**Visit, Phone, Email**	**On going Discussions about PET CSM Activities**
Bob Bernard	**ERDC CHL**	**CSM**	**Weed**	**Visit, Phone, Email**	**Discussions about Challenge Project**
Charlie Berger	**ERDC CHL**	**CSM**	**Weed**	**Visit, Phone, Email**	**Discussions about Challenge Project**

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
CWO					
Rebecca Brooks Lihwa Lin	ERDC CHL	CWO	Wornom	Visit, E-mail	Obtained wind fields for Hurricane Luis Simulation
Bob Jensen	ERDC CHL	CWO	Wornom	Visit, E-mail	Discussions concerning coupled runs of the SWAN and WAM wave models
Erick Rogers Larry Hsu James Kaihatu	NRL Stennis	CWO	Wornom Welsh	Visit, ERDC PET Workshop, E-mail	Discussions concerning SWAN wave model applications
Alan Wallcraft	NRL Stennis	CWO	Wornom	Visit, E-mail	Evaluation of the PThreads multiprocessing package
Don Resio Barbara Tracy	ERDC CHL	CWO	Wornom	Visit, E-mail	Discussions concerning the FBM wave-wave interaction model
Jane Smith Ann Sherlock	ERDC CHL	CWO	Wornom	Visit, E-mail	Discussions concerning STWAVE wave model applications
Joe Gailani Jim Clausner Norm Sheffner Bob Jensen Rebecca Brooks	ERDC CHL	CWO	Welsh Sadayappan	Visit, E-mail	Discussions concerning COMAPS Focused Effort activities
Don Resio Jane Smith	ERDC CHL	CWO	Bedford Welsh	Telephone, E-mail	Discussions concerning STWAVE wave model application

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
CWO					
Nolan Raphelt	**ERDC CHL**	**CWO**	**Welsh**	**E-mail**	**Notification of possible pre-existing CH3D-SED coding errors**

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
EQM					
Charlie Berger	**ERDC CHL**	**EQM**	**Luong, Parr, Jenkins, Dawson**	**Visit, Email**	**Discussed INLib, UTPROJ3D, and discontinuous of Galerkin Method**
Fred Tracy	**ERDC MSRC**	**EQM**	**Wheeler, Dawson, Luong**	**Visit**	**Discussed Status of Projects**
Rao Vemulakonda	**ERDC CHL**	**EQM**	**Luong**	**Visit, Email**	**Discussed CH3D-Z Multiblock Grid**
Stacy Howington	**ERDC CHL**	**EQM**	**Wheeler, Dawson, Luong, Jenkins**	**Visit, Email**	**Discussed possible Incorporation of DG into ADH and Two-phase Models**
Bob Bernard	**ERDC CHL**	**EQM**	**Wheeler, Dawson, Luong**	**Visit, Email**	**Discussed CH3D-Z Multiblock Grid**
Mark Dortch	**ERDC EL**	**EQM**	**Luong**	**Visit, Email, Phone**	**Discussed Support for NGLI Project**

Table 3
ERDC MSRC User Contacts

CEWES User	User Site	CTA	ERDC PET Team Member	Mode of Contact	Purpose/Result
EQM					
Ron Heath	ERDC CHL	EQM	Luong, Parr	Visit, Email, Phone	Discussed CH3D-Z Domain Decomposition
Jane Smith	ERDC CHL	EQM	Luong	Email	Workshop and EQM Support
John Peters	ERDC GL	EQM	Luong	Email	Workshop and EQM Support
Jackie Hallberg	ERDC CHL	EQM	Luong, Jenkins	Visit, Email	Workshop and EQM Support
Gary Brown	ERDC CHL	EQM	Luong, Parr	Visit, Email	Discussed UTPROJ3D Related Project
Bernard Hsieh	ERDC CHL	EQM	Luong	Email	Workshop and EQM Support
Billy Johnson	ERDC CHL	EQM	Luong, Parr	Visit, Phone, Email	Discussed CH3D-Z Project
Larry Hsu	NAVO MSRC	CWO	Luong	Visit, Email	Workshop and NGLI Support
Matt Bettencourt	CHL-Stennis	EQM	Wheeler, Dawson, Luong	Visit, Phone, Email	Workshop and NGLI Support
Michael Brooking	CHL-Stennis	EQM	Wheeler, Dawson, Luong	Visit, Phone, Email	Support CWO at NAVO MSRC

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
EQM					
Pete Gruzinskas	**NAVO**	**EQM**	**Wheeler, Dawson, Luong**	**Visit, Phone, Email**	**Support CWO at NAVO MSRC**
Carl Szczechowski	**NAVO**	**EQM**	**Wheeler, Dawson, Luong**	**Visit, Phone, Email**	**Workshop and Support NGLI Project**
Paul Martin	**NRL Stennis**	**CWO**	**Wheeler, Dawson, Luong**	**Visit, Email**	**Workshop and Support CWO at NAVO MSRC**
Alan Wallcraft	**NRL Stennis**	**CWO**	**Wheeler, Dawson, Luong**	**Visit, Email**	**Workshop and Support CWO at NAVO MSRC**
John Harding	**NRL Stennis**	**CWO**	**Luong**	**Email**	**Workshop and Support CWO at NAVO MSRC**
Robert Rhodes	**NRL Stennis**	**CWO**	**Luong**	**Email**	**Workshop and Support CWO at NAVO MSRC**
George Heburn	**NRL Stennis**	**CWO**	**Luong, Dawson, Wheeler**	**Email**	**Workshop and Support CWO at NAVO MSRC**
John Blaha	**NAVO MSRC**	**EQM**	**Wheeler, Luong**	**Email**	**Support NGLI Project**

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
EQM					
Jeffery Holland	**ERDC CHL**	**EQM**	**McGehee**	**Visit**	**Technical Discussions**
Dave Richards	**ERDC CHL**	**EQM**	**McGehee**	**Visit**	**Technical Discussions**
Barbara Donnell	**ERDC CHL**	**EQM**	**McGehee**	**Visit**	**Technical Discussions**
Stacy Howington	**ERDC CHL**	**EQM**	**McGehee**	**Visit**	**Technical Discussions**
Fred Tracy	**ERDC MSRC**	**EQM**	**McGehee**	**Visit**	**Technical Discussions**
Kent Eschenberg	**ERDC MSRC**	**EQM**	**McAdams**	**Email**	**Technical Discussions**

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
SPPT					
Robert Dees Henno Allik	**BBN Tech**	**EQM**	**Shirley Moore Dorian Arnold**	**Visit**	**Deliver and Demonstrate NetSolve Implementation of Analysis Tools**
Robert Maier	**Army HPC Research Center**	**EQM**	**David Cronk**	**Phone, Email**	**Discussed the Addition of MPI-I/O Support to EQM Challenge Code LBMPI**

Table 3 ERDC MSRC User Contacts					
CEWES User	**User Site**	**CTA**	**ERDC PET Team Member**	**Mode of Contact**	**Purpose/Result**
SV					
Ron Heath	**ERDC CHL**	**EQM**	**Folk**	**Email, Phone**	**Discuss HDF Work**
Mark Noel	**ERDC EL**	**EQM**	**Shih**	**Email, Phone**	**Discuss Visualization Work**
Carl Cerco	**ERDC EL**	**EQM**	**Shih**	**Email, Phone**	**Discuss Visualization Work**

Table 4
Training Courses

Course Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees
Note: Attendees Broken Down By: (On-Site MSRC users, Off-Site MSRC users, PET/integrator personnel, HBCU/MI personnel, other)						
Mesoscale Atmospheric Models	ERDC MSRC	2 Days	Ohio State	David Welsh Stephen Wornom	Workshop	12(8,0,3,1,0)
Lectures in CFD	ERDC MSRC	1 Day	MSU	Bharat Soni	Class, Tango	14(2,7,5,0,0)
Quantitative Performance Analysis and the PAPI Library	ERDC MSRC	1 Day	Tennessee	Philip Mucci	Class	7(0,0,7,0,0)
Parallel Debugging and Performance Analysis Tools	ERDC MSRC	2 Days	Rice	Clay Breshears	Class	7(2,0,4,1,0)
Developing and Optimizing Scientific Applications on IBM Power3 SMP Systems	ERDC MSRC	3 Days	IBM	David Klepacki Eric Myra	Class	13(1,0,12,0,0)
Using the SGI Origin Systems	ERDC MSRC	2 Days	OSC	Troy Baer	Class, Webcast	9(2,1,6,0,0)
Using the Cray T3E	ERDC MSRC	2 Days	OSC	David Ennis	Class, Webcast	4(0,0,4,0,0)
Reactive Transport on Unstructured Grids	ERDC MSRC	1 Day	Texas	Mary Wheeler	Class	21(14,0,7,0,0)
SHAMRC Users Course	ERDC MSRC	5 Days	ARA	Charles Needham Joseph Crepeau	Class	7(5,0,2,0,0)

Table 4
Training Courses

Course Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees
Note: Attendees Broken Down By: (On-Site MSRC users, Off-Site MSRC users, PET/integrator personnel, HBCU/MI personnel, other)						
Pthreads Tutorial	ERDC MSRC	1 Day	Rice	Richard Hanson	Class	10(3,0,7,0,0)
Introduction to the SWAN Wave Model	ERDC MSRC	2 Days	Ohio State	Keith Bedford Stephen Wornom	Workshop	14(3,7,4,0,0)
Multilevel Parallel Programming	AEDC	2 Days	OSC	David Ennis	Class	24(0,24,0,0,0)
Advanced ModSAF	ERDC MSRC	5 Days	Sagacitech	Vicky Rowley	Class	14(7,7,0,0,0)
Tutorial on Collaboration and Communication Technology	ERDC MSRC	1 Day	Florida State	Geoffrey Fox	Class	13(5,2,6,0,0)
Multiphysics Workshop	ERDC MSRC	1 Day	Texas	Mary Wheeler Phu Luong	Class	12(4,3,3,1,1)
SPEEDES Tutorial	ERDC MSRC	1 Day	Syracuse	Wojtek Furmanski	Class	7(1,0,6,0,0)
ALE Methodology	ERDC MSRC	1 Day	Texas	David Littlefield	Class	6(5,0,1,0,0)

Table 5
Training Courses & Seminars at HBCU/MIs

Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees
*Number of Attendees Broken Down by (Undergraduates, Graduate, Faculty/Staff)						
Spring 2000						
Advanced Visualization Systems Training Workshop	JSU	1 Day	JSU	Chuck Patrick	Scientific Visualization Class	4(0,0,4)
Fall 2000						
CSC 499 Java Programming Language	JSU	16 Weeks	JSU	Qutaibah Malluhi	Web-Based Class	11(11,0,0)
Spring 2001						
Alias/WaveFront, Maya3, Graphics & Animation Workshop	JSU	2 Days	JSU	Chuck Patrick	Scientific Visualization Class	13(7,0,6)

Table 6
HBCU/MI Students Impacted

Student	Level	Major	University	Activity
2000 Summer Institute				
Ceesay Alhagie	Junior	Computer Science	Rust College	Summer Institute
Deavin Banks	Sophomore	Computer Science	Jackson State	Summer Institute
Marlon Brooks	Senior	Computer Science	Jackson State	Summer Institute
Ingrid Clay	Sophomore	Computer Science	Xavier	Summer Institute
Cottrell Davis	Sophomore	Computer Science	Dillard	Summer Institute
Corey Dixon	Junior	Computer Science	Rust College	Summer Institute
Marc Farrow	Junior	Computer Science	Rust College	Summer Institute
Aisha Gates	Junior	Computer Science	Jackson State	Summer Institute
Tamika Greenwood	Sophomore	Physics	Jackson State	Summer Institute
Jeremy Hardy	Junior	Computer Technology	Jackson State	Summer Institute

Table 6 HBCU/MI Students Impacted				
Student	**Level**	**Major**	**University**	**Activity**
2000 Summer Institute				
Alfred James	**Junior**	**Computer & Information Technology**	**Langston**	**Summer Institute**
Nicole Jones	**Sophomore**	**Computer Science**	**Rust College**	**Summer Institute**
Veronica Jones	**Junior**	**Computer Science**	**Rust College**	**Summer Institute**
Johnson Sonji	**Sophomore**	**Physics**	**Jackson State**	**Summer Institute**
Sylayman Mbenga	**Junior**	**Mathematics & Computer Science**	**Rust College**	**Summer Institute**
Torsha McElroy	**Junior**	**Biology**	**Tuskegee Institute**	**Summer Institute**
Olivia Moton	**Sophomore**	**Mathematics**	**Jackson State**	**Summer Institute**
Fareedah Sabree	**Sophomore**	**Computer Science**	**Dillard**	**Summer Institute**
Latoya Taylor	**Sophomore**	**Computer Science**	**Jackson State**	**Summer Institute**
Cheryl Townsend	**Sophomore**	**Computer Science**	**Mississippi Valley State**	**Summer Institute**

Table 6
HBCU/MI Students Impacted

Student	Level	Major	University	Activity
Spring 2000 Advanced Visualization Systems Training Workshop				
Jennifer R. Banks	Staff	HPVCI/Information Technology	Jackson State	Visualization Workshop
Hailong Li	Staff	HPVCI/Information Technology	Jackson State	Visualization Workshop
Monika Rabarison	Staff	HPVCI/Information Technology	Jackson State	Visualization Workshop
Fall 2000 JSU CSC 499 Java Programming Language				
Ronald Anderson II	Undergraduate	Computer Science	Jackson State	College Course
Marlon Brooks	Undergraduate	Computer Science	Jackson State	College Course
Taheerah Fulgham	Undergraduate	Computer Science	Jackson State	College Course
Shawana Hawthorne	Undergraduate	Computer Science	Jackson State	College Course
Lail Hossain	Undergraduate	Computer Science	Jackson State	College Course
Gerardl Howard	Undergraduate	Computer Science	Jackson State	College Course

Table 6 HBCU/MI Students Impacted				
Student	**Level**	**Major**	**University**	**Activity**
Fall 2000 JSU CSC 499 Java Programming Language				
Christian Kendrick	**Undergraduate**	**Computer Science**	**Jackson State**	**College Course**
Zhi Lin	**Undergraduate**	**Computer Science**	**Jackson State**	**College Course**
Sherar N. Mohammad	**Undergraduate**	**Computer Science**	**Jackson State**	**College Course**
Kimani Price	**Undergraduate**	**Computer Science**	**Jackson State**	**College Course**
Timothy Strickland	**Undergraduate**	**Computer Science**	**Jackson State**	**College Course**
Spring 2001 Alias/WaveFront, Maya3, Graphics & Animation Workshop				
Jennifer Banks	**Staff**	**HPVCI/Information Technology**	**Jackson State**	**Visualization Workshop**
Alvin Blue	**Student**	**HPVCI/Information Technology**	**Jackson State**	**Visualization Workshop**
Charles Brice	**Student**	**HPVCI/Information Technology**	**Jackson State**	**Visualization Workshop**
Crystal Holmes	**Student**	**HPVCI/Information Technology**	**Jackson State**	**Visualization Workshop**

Table 6
HBCU/MI Students Impacted

Student	Level	Major	University	Activity
Spring 2001 Alias/WaveFront, Maya3, Graphics & Animation Workshop				
Hailong Li	Student	HPVCI/Information Technology	Jackson State	Visualization Workshop
Monika Rabarison	Staff	HPVCI/Information Technology	Jackson State	Visualization Workshop
Brenda K. Rascoe	Staff	DoD Modernization	Jackson State	Visualization Workshop
Veries Seals	Student	HPVCI/Information Technology	Jackson State	Visualization Workshop
Cornelius Toole	Student	HPVCI/Information Technology	Jackson State	Visualization Workshop
Albert Williams	Student	HPVCI/Information Technology	Jackson State	Visualization Workshop
Torrence Williams	Student	HPVCI/Information Technology	Jackson State	Visualization Workshop
John Young	Staff	HPVCI/Information Technology	Jackson State	Visualization Workshop